ICNC2024

19th International Conference on Numerical Combustion

Kyoto, Japan

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Book of Abstracts

Welcome Note

Carbon dioxide (CO_2) is the largest contributor to greenhouse gases, and the majority of its emissions originate from the combustion of fossil fuels such as coal, oil and natural gas. Therefore, countermeasures to the impact of CO_2 are urgently required. Energy that is directly converted from wind and sunlight, that is renewable energy has gained attention in recent years as an alternative to the energy obtained through burning of fossil fuels. However, their global application is time-consuming and demanding. Therefore, to obtain clean and efficient energy during combustion, research has been actively conducted on methods for burning carbon-free fuels such as hydrogen (H_2) and ammonia (NH_3), which do not contribute to net CO_2 emissions. H_2 and NH_3 can be produced ultimately from the electrolysis of water using renewable energy, increasing the expectations for the realization of carbon-free combustion systems used in energy production devices. Furthermore, improved safety, reduced costs, and reduced emissions of environmental pollutants from aircraft engines are strongly desired. Although the use of aircrafts temporarily declined owing to the impact of the COVID-19 pandemic, it is expected to increase in the future. The usage of rockets is also expected to increase as these are at the heart of the space industry for important infrastructure related to the future social, economic, and security activities. In addition, precise prediction and control of wildland fires have been serious challenges. Therefore, further understanding of combustion physics and development of advanced combustion technologies are becoming increasingly important.

Combustion is an extremely complex phenomenon in which reactions involving hundreds of chemical species occur over thousands to tens of thousands of steps at most, in a turbulent flow field, accompanied by heat generation. Therefore, numerical simulations are essential for elucidating the mechanisms, developing combustion systems that efficiently utilize these principles, and selecting optimal operating conditions.

The International Conference on Numerical Combustion (ICNC) is a major international conference in the combustion field. The ICNC has been held biennially for exchanging information and improving the level of research on the science and technology of combustion through multilateral exchange. Locations for the ICNC were in Europe and the United States; the recent locations for ICNC include Avignon (France) in 2015, Orlando (U.S.A.) in 2017, Aachen (Germany) in 2019, and San Diego (U.S.A.) in 2022 (postponed by one year because of COVID-19).

The 19th ICNC in 2024 (ICNC2024) will be held in Kyoto, Japan: the first non-western hosting venue for the conference. The ICNC2024 will be held with the full support of The Combustion Institute and its Japan section. Kyoto city is not only the cultural capital of Japan and a major tourist destination, but also famous as the place where the Kyoto Protocol regarding the reduction of greenhouse gas emissions was first adopted on 11 December, 1997. At the ICNC2024, a total of 20 mini-symposia will be held, and 4 invited lectures and more than 470 oral presentations will be delivered in the mini-symposia and the general tracks. We sincerely hope that researchers and engineers worldwide working in this field will come together and join in lively discussions and information exchange on both basic and applied research.

Greetings, on behalf of the Organizing Committee

Ryoichi Kurose, Mamoru Tanahashi and Yasuhiro Mizobuchi

Invited Speaker

Hideaki Kobayashi
Tohoku University, Japan

Fundamentals and Applications of Ammonia Combustion for Carbon Neutrality

Abstract

Ammonia is one of the most fundamental chemicals. It is an old and new fuel whose potential for fuel use has already been investigated for more than 80 years. It is currently a candidate for decarbonization fuels alongside hydrogen towards carbon neutrality. Basic research and technological development have intensified rapidly within the last decade. The focus on ammonia or hydrogen depends on the geopolitical conditions affecting the availability of renewable energy for production and the cost of transportation of these fuels. The huge demand for energy in the power generation, industrial and maritime sectors means that the expected future distribution volumes are also huge. This has created international competition as well as international cooperation to build global supply chains.

Ammonia and hydrogen can be regarded as family fuels with interdependencies in the production process as well as commonalities in terms of decarbonization fuels, but their combustion characteristics are completely different. Hydrogen has very high reactivity and ignitability and NOx production is due to thermal NO, whereas ammonia has very low reactivity and ignitability and NOx production is due to fuel NO. Modern combustion science, i.e. detailed reaction mechanism construction, large-scale numerical analysis methods and laser diagnostics, play an important role in solving these problems. In addition, the use of ammonia as a fuel in a high-pressure environment, such as large gas turbines and marine engines, requires the technological development to inject liquid ammonia and burn. New basic research is needed on liquid ammonia spray formation and combustion, and low NOx combustion methods under high pressure. The lecture describes the progress in technological development towards the social implementation of ammonia combustion systems, as well as basic research efforts, particularly in ammonia gas turbine combustion.

Short Biography

Hideaki Kobayashi is a Research Professor at Tohoku University, Japan. He is involved in projects on basic ammonia combustion, development of ammonia gas turbines and industrial furnaces using ammonia, with a view to decarbonization and fuel conversion in the energy and industrial sectors. He also works on national and international project evaluations and international standardization on ammonia utilization as a fuel. Professor Kobayashi has been involved in research on fundamental processes of combustion phenomena in extreme environments, such as high-pressure turbulent premixed combustion, supersonic combustion, microgravity combustion and low-oxygen, high-temperature air combustion. He served as the team leader of the ammonia direct combustion research in the national project SIP "Energy Carriers", which ran for five years from 2014.

Professor Kobayashi completed his master degree at Tohoku University in 1983 and became an assistant professor at the university, where he obtained his PhD in 1991. After working as an associate professor, he became a professor at Institute of Fluid Science, Tohoku University in 2003. He served as Program Co-Chair of the 32nd International Symposium on Combustion in 2008, President of Combustion Society of Japan from 2015 to 2017 and Vice-President of The Combustion Institute from 2016 to 2020. He received The Commendation for Science and Technology by The Minister of Education, Culture, Sports, Science in 2017 and Technology and The Thermal Engineering Award for Outstanding Academic Contribution by The Japan Society of Mechanical Engineers in the same year. In 2018 he was honored as a Fellow of The Combustion Institute and in 2022 he was awarded The Bernard Lewis Gold Medal.

Invited Speaker

Terese Løvås

Norwegian University of Science and Technology, Norway

Do the Thermodynamic Properties of New Fuels Challenge the Current State-of-the-art Modeling?

Abstract

After the UN Climate Meeting COP28, there is little doubt that we are experiencing the "beginning of the end" of the fossil fuel era. Nearly every country in the world is committed to transitioning away from fossil fuels. Other critical key outcomes from the meeting included a commitment to triple the renewable energy capacity by 2030. The combustion community has, for a while now, already devoted much research to address these matters with a focus on understanding and enabling the usage of low-carbon or carbon-free fuels such as methanol, hydrogen, and ammonia in combustion devices. It has been argued that combustion as a means of energy production is not the obstacle to climate change but rather the fuel used.

However, the advances in combustion technology that are now becoming state-of-the-art represent a challenge when introducing new fuels to existing combustion technology. High pressure direct injection is a common strategy for fuel delivery systems in internal combustion engines, whereas reactivity controlled compression ignition (RCCI) and direct dual fuel stratification (DDFS) are being explored to achieve satisfactory engine performance with effective control combustion to minimize emissions. Moderate or Intense Low oxygen Dilution (MILD) combustion technology is yet another strategy is another promising strategy for clean and efficient combustion.

These new approaches do, however, require a fundamental understanding of the fuel's behavior under demanding conditions. Differences in boiling point and latent heat of vaporization give rise to phenomena such as cavitation or flash boiling in the injection system and cause spray development and evaporation inside the combustion chamber to deviate significantly from the familiar hydrocarbon fuel sprays. It is worth noting that thermodynamic properties of ammonia are usually found in refrigeration tables. Many modeling approaches currently widely used in combustion research do not satisfactorily account for these phenomena, and existing models need to be further adapted and extended for a broader range of thermodynamic properties.

In the lecture, an overview of the most critical properties of concern will be given alongside a description of their importance for phenomena such as vaporization, cavitation, and flash boiling. Existing models will be reviewed to explore areas of development. Comparison with experiments will allow us to identify the importance of such model development to capture new fuels' applicability in current combustion devices correctly.

Short Biography

Dr. Løvås completed her master's in relativistic astrophysics at the Niels Bohr Institute at the University of Copenhagen in Denmark in 1998. She obtained her doctorate in combustion physics at Lund University in Sweden in 2002, focusing on chemical kinetics and model reduction. She also holds a master's degree from the University of Cambridge.

Dr. Løvås has, among other things, worked as a researcher and lecturer in energy technologies at Queen Mary University of London and as a researcher at the University of Cambridge. She has been a Fellow in Engineering at Churchill College, Cambridge.

Since 2009, Løvås has been a Professor and group leader for the thermal energy research group at the Department of Energy and Process Engineering at the Norwegian University of Science and Technology, NTNU. Here, she has also extended her research towards solid fuels. She has led several research projects on ammonia and hydrogen combustion for marine applications in recent years. In August 2017, Dr. Løvås took the position of Head of the Department of Energy and Process Engineering at NTNU. She became the first female head in the department's history.

Dr. Løvås has been teaching thermodynamics and combustion science at various universities and has authored more than 90 peer-reviewed journal papers. She has participated in many collaborative projects at the national and international levels. She is a member of the Board of Directors of the Combustion Institute and has been joint Editor of the Proceedings of the Combustion Institute since 2020. From 2011-2017, she was president of the Scandinavian Nordic section at the international research community Combustion Institute, and from 2015-2023, she took over as president of the Federation of European sections of the same research community. She is a board member of the Swedish national research program and strategic research center CECOST, Center for Combustion Science and Technology. In addition, she was a board member for the national infrastructure provider for computational science in Norway UNINETT Sigma2 AS.

Invited Speaker

Matthias Ihme
Stanford University, USA

Machine-learning for Combustion: Opportunities and Challenges

Abstract

Combustion and energy conversion play critical roles in all facets of environmental and technological applications, including the utilization of sustainable energy sources for power-generation, the mitigation of harm from wildfire hazards, or the reductions of emissions from furnaces and industrial processing systems. Computational and mathematical tools have long been crucial in combustion research in the form of high-fidelity simulations, dynamical-system modeling, and data analytics. With the advent of data-driven methods, machine learning (ML) offers numerous new opportunities for predictive modeling, improving existing research methods, and extracting new knowledge from data. In this presentation, we discuss recent progress on how ML can impact the field of combustion and energy conversion and discuss the need for injection physical principle and domain knowledge for successful machine-learning application in combustion. Specifically, instead of image and textual data seen in many ML applications, combustion ML learns from data extracted from large-scale simulations, high-resolution experiments, and sensors, which can introduce challenges tied to dimensionality, sparsity, and scarcity. Here, domain knowledge and expertise can help alleviate these challenges, with the additional benefit of introducing physical constraints seen in real-world problems. We discuss these knowledge-guided strategies and further requirements in combustion ML linked to interpretability, uncertainty quantification, robustness, consistency, and benchmark datasets.

Short Biography

Matthias Ihme is Professor in the Department of Mechanical Engineering at Stanford and the Department of Photon Sciences at SLAC National Accelerator Laboratory. He holds a BSc. degree in Mechanical Engineering, a MSc. degree in Computational Engineering, and a Ph.D. in Mechanical Engineering. His research interests are broadly on the computational modeling of reacting flows, the development of numerical methods, and the investigation of advanced energy conversion concepts and molecular processes. He is a recipient of the NSF CAREER Award (2009), the ONR Young Investigator Award (2010), the AFOSR Young Investigator Award (2010), the NASA Early Career Faculty Award (2015), the Hiroshi Tsuji Early Career Research Award (2017), and the Bessel Award of Alexander von Humboldt Foundation (2021).

Invited Speaker

Epaminondas Mastorakos
University of Cambridge, UK

Advances in Simulations of Dual-fuel Combustion

Abstract

In this talk, the Doubly-Conditioned Moment Closure sub-grid combustion model is presented and discussed in the context of recent simulations of lifted spray flames, dual-fuel swirl flames, and diesel-ignited ammonia flames. The seminar discusses the strengths and limitations of the approach and includes a review of salient features of dual-fuel flames and the challenges associated with their modelling. Comparison with other modelling approaches for this problem is attempted.

Short Biography

Epaminondas Mastorakos is the Hopkinson/ICI Professor of Applied Thermodynamics at the Engineering Department, University of Cambridge. He joined Cambridge in 2000 after education at Imperial College and Cornell University and post-doctoral appointments in Keio University (Yokohama, Japan), Institut Francais du Petrole (Paris, France), and the Institute for High Temperature Process (Patras, Greece).

He has experience with fuels, energy, combustion, atmospheric chemistry, aerosols, the fluid mechanics of shale oil and gas, forest fires, and energy systems for aviation and shipping. His lab has received funding from industry, the EU, Singapore's NRF and UK's EPSRC on a range of topics, with significant activity on gas turbine and diesel engine combustion, and aviation and shipping decarbonisation. He is currently the Combustion Research Coordinator in the Rolls-Royce / Cambridge University Gas Turbine Partnership. His papers have received numerous prizes from the Combustion Institute and the American Society of Mechanical Engineers and he has been elected Fellow of the Combustion Institute (2018), Fellow of the UK Institute of Mechanical Engineers (2019), and Fellow of the Royal Academy of Engineering (2022).

Concerning numerical combustion, he has focused his work on implementing the Conditional Moment Closure and its variants to LES of various flames of practical relevance such as gas turbine combustors.

MS01 Reaction Kinetics of Carbon-Neutral Fuels

Organizers: Akira Miyoshi[1], Yasuyuki Sakai[2]

[1]Hiroshima University, [2]Ibaraki University

MS01 Reaction Kinetics of Carbon-Neutral Fuels

Chair: Akira Miyoshi
Co-Chair: Yasuyuki Sakai
Wednesday, May 8; 15:30 - 16:50; Room J

Combustion Properties of Alcohol Fuels

Akira Miyoshi
Hiroshima University, Japan

In order to achieve the carbon-neutral society, our energy sources should shift toward biofuel and synthetic fuels. Alcohols, methanol and ethanol, are the promising alternative fuels for gasoline either by neat fuel or drop-in fuels for existing petroleum fuels. Using their chemical kinetic models, anti-knock properties and laminar burning velocities has been well confirmed. In the present study, the extinction flame stretch, which largely determines the lean limit of the SI super lean combustion and ignition problems at cold start, has been extensively investigated by the numerical simulation of counter-propagating premixed flame and nitrogen stream. The non-additive anti-knock effect (octane hyper-boost) of ethanol to alkanes has been also investigated by the autoignition simulations.

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Development of High-Performance Formula 1 Fuel Component and its Carbon-Neutralization

Kohtarro Hashimoto
Honda R & D Co. Ltd., Japan

High-performance component of Formula 1 (F1) fuel was developed using chemical reaction calculations. Chemical reaction models of various hydrocarbons were created using KUCRS. Ignition timing of these hydrocarbons under the pressure conditions of the combustion chamber of F1 engine were calculated using Ansys Chemkin. As the candidate for high performance components having anti-knock properties was found, it has been used for F1 fuel component from 2019 Japan Grand Prix (GP). Next, carbon-neutralization of this high-performance component was attempted. Renewable hydrogen and biomass as carbon sources were used to produce e-methanol. In addition to e-methanol, biochemical produced from second-generation biomass and chemicals were used to produce this high-performance component. As a result, this high-performance component was composed of 58.5% of renewable carbon. The F1 fuel mixed with this component was used for in the 2021 Saudi Arabia GP and Abu Dhabi GP for Honda's power unit.

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A Chemical Kinetic Study on the Autoignition Mechanism of Ammonia/hydrocarbon mixtures

Yasuyuki Sakai[1], Takahiro Sako[2], Sekai Miyamoto[3], Takahiro Yamaguchi[3], Hisashi Nakamura[4]
[1]Ibaraki University, Japan, [2]Osaka Gas Co.,Ltd., Japan, [3]Kawasaki Heavy Industries, Ltd, Japan, [4]Tohoku University, Japan

The use of ammonia combustion is one way to contribute to the carbon neutralization of marine engines and industrial furnaces. During the transition period from hydrocarbon fuels derived from fossil resources to ammonia, various forms of ammonia combustion are envisioned such as natural gas/ammonia, light oil/ammonia, heavy oil/ammonia co-firing, and pure ammonia firing. The present study reports an analysis of the combustion reaction mechanism of hydrocarbon/ammonia mixtures by using a detailed chemical kinetics mechanism developed by authors. Starting from the reaction mechanism of hydrocarbon mixtures (methane, ethane, propane, n-butane, and isobutane), an ammonia combustion mechanism and mechanism of the intermediate species containing both carbon and nitrogen atoms (CN, HCN, CH2NH2, etc.) produced during the combustion of hydrocarbon/ammonia mixture were added. The present mechanism includes 462 species and 2720 reactions. Ignition delay times and laminar flame velocities were used for the validations of our mechanism. Ignitability is suppressed under both high and low temperature conditions with increasing the amount of ammonia, however there is a region where ignitability of

ethane is enhanced at 60~90% ammonia mixture. A similar trend appears in the calculation results for methane/ammonia mixtures, but not for propane/ammonia and butane/ammonia mixtures. We will give the analysis of these promotion/suppression effects in the presentation.

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Laminar burning velocity of ethanol/air premixed flame under lean conditions

Yuki Ito, Kento Masui, Taku Mizutani, **Hidefumi Kataoka**, Daisuke Segawa
Osaka Metropolitan University, Japan

Ethanol is derived from biomass and is a carbon-neutral fuel. The combustion experiments of ethanol/air mixture under lean conditions were conducted using a spherical combustion vessel. The laminar combustion velocity was derived from the obtained pressure history. Numerical calculations of a one-dimensional premixed ethanol/air flame were performed using a detailed reaction mechanism. The calculated laminar burning velocity was compared with the experimental results of laminar burning velocity.

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MS02 Direct numerical simulations, analysis, and modeling of premixed hydrogen flames

Organizers: Heinz Pitsch[1], Mamoru Tanahashi[2], Andrew Aspden[3], Martin Rieth[4], Michael Gauding[1]

[1]RWTH Aachen University, [2]Tokyo Institute of Technology, [3]Newcastle University, [4]Sandia National Laboratories

MS02-1 Direct numerical simulations, analysis, and modeling of premixed hydrogen flames (1)

Chair: Thomas Howarth
Friday, May 10; 09:50 - 11:50; Room K

Thermodiffusively-unstable lean premixed hydrogen flames: Length scale effects and turbulent flame speed modelling

E. F. Hunt, **A. J. Aspden**
Newcastle University, United Kingdom

Burning hydrogen in a lean premixed mode can control high flame speeds, temperatures and emissions, but can result in thermodiffusively-unstable flames. Recent work [CNF111805] has demonstrated that two-dimensional freely-propagating flames can be well characterised with a stability parameter that arises from classical stability analysis [JFM489p179], and was then extended to three-dimensional freely-propagating and turbulent flames [CNF112811]. These two studies were restricted to relatively-small length scales. The present paper considers the influence of domain and integral length scales on local and global flame behaviour across a broad range of reactant (i.e. temperatures and pressures) and turbulence conditions (i.e. Karlovitz and Damkohler numbers). The general local flame behaviour (and moreover the local flame speed model from [CNF112811]) is demonstrated to be independent of length scale at a fixed Karlovitz number. Consequently, once thermodiffusive effects on the local flame speed have been accounted for, turbulent flame speeds are determined solely by flame surface area enhancement. A range of turbulent flame speed models are compared with the present simulation data and those in [CNF112811]. Limitations were found when evaluating turbulent flame speeds in the small domains inherent to DNS, which can be misinterpreted as "the bending effect". Comparisons are made varying fuel Lewis number from 0.35 to 2.0, which demonstrate contrasting behaviour, both locally (i.e. local flame speed and curvature dependence) and globally (i.e. flame surface area enhancement). Finally, consequences for the turbulent premixed regime diagram are discussed.

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DNS of a hydrogen flame interacting with homogeneous isotropic turbulence maintained by a deterministic force

Yifan Xu[1], Jian Fang[2], Zhen Lu[1], Xiaojun Gu[2], Zhi X. Chen[1]
[1]Peking University, China, [2]Science and Technology Facilities Council, United Kingdom

Studying the interplay between a hydrogen flame and turbulence is crucial for the advancement of next-generation carbon-neutral combustion systems. In our present work, we conduct a series of direct numerical simulations (DNS) to investigate the dynamics of a premixed hydrogen flame interacting with the compressible homogeneous isotropic turbulence (HIT) maintained by a deterministic force under different pressure and turbulence intensity. Under this particular forcing method applied to turbulence at large scales, the relationship between the forcing intensity and the resulting fluctuating velocity aligns well with the experimental results. In our study, we compare the statistics of turbulent burning velocity of hydrogen flames under different conditions and verify the common occurrence of bending effects at elevated pressures. To further explore the dynamics of the HIT-flame interaction and fully leverage the advantages of high-precision direct numerical simulations, we analyse several flame behaviours such as stretch and instability, as well as higher-order turbulence statistics such as skewness. The probability density function (PDF) for the tangential strain rate and curvature are displayed and the results indicate a strong correlation between the flame surface structure and the turbulence generated by the large-scale forcing.

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Effects of Reynolds number on thermodiffusive flame instabilities: Direct numerical simulations of turbulent lean hydrogen jet flames

Michael Gauding, Thomas Howarth, Lukas Berger, Heinz Pitsch
RWTH Aachen University, Germany

Lean premixed hydrogen/air flames are significantly affected by thermodiffusive instabilities. These originate from the disparity between heat and mass fluxes due to the low Lewis number of hydrogen and lead to significantly increased burning velocities. In turbulent flames, these effects persist and are even further amplified by synergistic interactions among turbulence and thermodiffusive instabilities.

In this work, the dependence of these synergistic interactions on the Reynolds number is quantitatively assessed via direct numerical simulations (DNS) of premixed hydrogen/air jet flames utilizing finite rate chemistry in a slot burner configuration. A fixed reactant condition is employed (equivalence ratio of 0.4, 1 bar, 298 K) and the jet slot width is increased to vary the jet Reynolds numbers between 5,500 and 22,000 while keeping the Karlovitz number constant. Global and surface-local statistics are retrieved to characterize the jet and turbulence-flame interaction. The dependence of thermodiffusive instabilities on the jet Reynolds number is analyzed through local curvature, strain and stretch rate, and flame morphology. Variations of the local reactivity, which are linked to the fluctuations of equivalence ratio, are analyzed. Strain effects are assessed by comparison with laminar counterflow flamelets.

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Direct Numerical Simulation of a Lean-Premixed Turbulent Swirling Hydrogen Flame

Abhishek Lakshman Pillai[1], Umair Ahmed[2], Nilanjan Chakraborty[2], Ryoichi Kurose[1]
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This study presents an analysis of turbulent combustion in an actual laboratory-scale lean-premixed (equivalence ratio = 0.45) low-swirl hydrogen flame using Direct Numerical Simulation (DNS). This lean-premixed hydrogen flame is stabilized using a Low-Swirl Burner (LSB) with a swirl number = 0.39. The DNS incorporates detailed chemical kinetics for hydrogen combustion and the differential diffusion of chemical species is considered by computing their respective diffusion velocities from the Maxwell-Stefan equation. The DNS domain is discretized by a non-uniform Cartesian grid with nearly 6 Billion grid points and is executed on the supercomputer Fugaku (RIKEN Japan) using 200,000 cores. Interrogation of the generated DNS database reveals that differential diffusion of reactants influences the local flame structure and causes the occurrence of localized super-adiabatic temperatures. While combustion is found to occur predominantly in the lean-premixed mode, some local regions of non-premixed combustion are found in the shear layers owing to mixture inhomogeneities arising from mixing and stratification effects in the hydrogen flame's swirling turbulent shear layers. Additionally, the DNS database is used to analyze the flame structure and the statistical behaviors of various quantities such as the mixture fraction, progress variable, temperature, chemical species concentrations, and surface density function in detail.

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DNS study of turbulent boundary layer flashback in parallel channel for lean hydrogen-air premixed flame

Reo Kai[1], Kotaro Yada[2], Kazuhiro Kinuta[2], Hiroaki Watanabe[1], Ryoichi Kurose[2]
[1]Kyushu University, Japan, [2]Kyoto University, Japan

To develop a stable hydrogen-fueled combustor with low NOx emissions, preventing and understanding the flashback of a lean hydrogen-air premixed flame is one of the most challenging. This study focuses on the flashback in the vicinity of the wall, namely the boundary layer flashback. To elucidate the mechanism of flashback of a lean hydrogen-air premixed flame in a turbulent boundary layer, a direct numerical simulation of turbulent boundary layer flashback in parallel channel for a lean hydrogen-air premixed flame at an equivalence ratio of 0.5, an unburnt gas temperature of 750 K, a pressure of 1 atm, and a friction Reynolds number of 180 is performed employing a detailed chemical reaction mechanism including 9 chemical species and 19 chemical reactions. The obtained results are analyzed to investigate the contributions of flame-flow interaction, flame-flame interaction, local equivalence ratio distribution, and thermal diffusive instability on the flashback behavior, such as flashback speed.

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DNS of a laboratory lean CH4/H2 low-swirl flame impinging on an inclined wall

Mohammadreza Nozari[1], Olivier Chabot[1], Sandeep Jella[2], Martin Vabre[1], Luming Fan[3], Marc Day[4], Patrizio Vena[3], Lucas Esclapez[5], **Bruno Savard**[1]

[1]Polytechnique Montréal, Canada, [2]Siemens Energy Canada Limited, Canada, [3]National Research Council Canada, Canada, [4]National Renewable Energy Laboratory, Canada, [5]National Renewable Energy Laboratory, United States

Direct numerical simulation of a lean swirling premixed H2/CH4 flame impinging on an inclined isothermal wall is performed. The case simulated is a laboratory flame with Reynolds number of 20,000 and Karlovitz number of 300. The fuel/air mixture consists of 70% hydrogen and 30% methane with equivalence ratio of 0.41. The simulation results are compared with experimental results from OHx-CH2O PLIF and stereo-PIV measurements. Consistently, the flame features a bowl-shape stabilization, with a corrugated, continuous flame front at the leading edge, followed by highly fragmented reaction zones downstream. A remarkably large cloud of CH2O and CO is formed downstream of the quenching point, also observed experimentally. The simulation results indicate that the cloud is the result of incomplete methane combustion caused by the stabilization of ultra-lean H2/CH4 reaction zones in strong shear layers. These reaction zones can sustain mean strain rates significantly larger than the 1D extinction strain rate. The role of wall heat loss on the flame stabilization and flame structure in phase space is also presented.

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MS02-2 Direct numerical simulations, analysis, and modeling of premixed hydrogen flames (2)

Chair: Martin Rieth
Friday, May 10; 13:00 - 15:00; Room K

DNS on flame structure and species distribution of a partially premixed steam-diluted oxygen/hydrogen combustion with inclining impinging jets geometry

Shan Jiang[1], Ye Wang[1], Masayasu Shimura[2], Mamoru Tanahashi[1]

[1]Tokyo Institute of Technology, Japan, [2]National Institute of Advanced Industrial Science and Technology, Japan

We conducted direct numerical simulations (DNSs) to investigate the flame structure, mixing properties as well as distribution of chemical species in a partially premixed steam-diluted oxygen/hydrogen combustion with inclining impinging jets geometry. It was found that the distance between jet nozzle groups poses significant influences by enhancing the interaction between neighboring flow fields and flame in the upstream region. Specifically, closer proximity of nozzle groups corresponds to a more extensive concentration of hydrogen upstream, along with a more intense recirculation in the domain between hydrogen nozzles. The upstream concentration of hydrogen may be attributed to the recirculation domain continuously transporting unburnt gases upstream. Furthermore, we observed that under smaller hydrogen nozzle spacings, the flames from adjacent groups of nozzles merges together and tends to be closer to the upstream region. Additionally, analysis using the Normalized Flame Index (NFI) revealed that the typical triple flame structure was no longer present under shorter nozzle group distances. The mixture in both premixed and non-premixed modes is more fragmented and distributed near the jet impinging points in the upstream part, compared to cases with larger nozzle group distances.

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Near-wall dynamics of V-shape hydrogen-air flame in a turbulent channel flow

Ye Wang, Mamoru Tanahashi
Tokyo Institute of Technology, Japan

The correlation between three-dimensional geometric structure and near-wall dynamics of turbulent hydrogen flame has been studied using direct numerical simulation

with detailed chemistry, considering the V-shape flame in a turbulent channel flow. The principal curvatures (k1, k2) and the local fuel consumption speed of each flame element are evaluated. The results show that, the influence of the wall is predominant in shaping the flame geometry in the buffer layer and viscus sublayer of near-wall turbulence, resulting in near-wall flames that are primarily cylindrical and convex towards either the burned or unburned side. Additionally, it is found that the local fuel consumption speed is not solely reliant on the flame's mean curvature but also on its principal curvatures: flame elements with identical mean curvature values but larger differences between k1 and k2 statistically exhibit higher fuel consumption speeds. This is different from the previous findings of the turbulent flame free of wall. The current study highlights the critical role of the three-dimensional geometry and principal curvatures to the near-wall flame reactions and proportions, which should be considered in the future modelling of near-wall turbulent premixed hydrogen combustion.

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Inducing Spiky Flame Fronts in Lean Hydrogen Flames through Expansion Waves

Samir Boset Rojas Chavez[1], Hongxia Yang[2], Kevin Cheevers[2], Deanna Lacoste[1], Matei Radulescu[2]

[1]King Abdullah University of Science and Technology, Saudi Arabia, [2]University of Ottawa, Canada

Hydrogen lean flames exhibit a fractal-like propagation, where larger cells encompass smaller, similar cells within the flame front. This structure results in cell intersections leaving behind funnels of unburned gases. Recent studies have highlighted the role of expansion waves in either accelerating burning velocity or quenching flames, depending on the expansion ratio and the wave's propagation direction relative to the flame (i.e., from burned to fresh gases or vice versa). Our study explores a novel effect of expansion waves on lean hydrogen-air flames (φ=0.3). We employed reactive Navier-Stokes equations in a two-dimensional domain, supplemented by cylindrical Hele-Shaw configuration experiments. A central shock tube in the Hele-Shaw setup generates expansion waves moving from burned to fresh gases. Our findings reveal an immediate cell flipping post-expansion wave interaction, followed by a distorted, spiky flame front formed by the combination of cell flipping and unburned gas funnels.

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On the behaviour of Reynolds stresses and their dissipation rates during boundary layer flashback of a rich hydrogen-air premixed flame within a turbulent channel flow

Umair Ahmed[1], Abhishek Pillai[2], Nilanjan Chakraborty[3], Ryoichi Kurose[4]

[1]Newcastle Univeristy, United Kingdom, [2]Kyoto University, Japan, [3]Newcastle University, United Kingdom, [4]Kyoto Univeristy, Japan

A Direct Numerical Simulation (DNS) database for boundary layer flashback of hydrogen-air premixed flame in a turbulent channel flow has been utilised to investigate the interrelation between Reynolds stresses and their dissipation rates. The Reynolds stresses and their dissipation rates have been found to exhibit significant deviations during boundary layer flashback when compared with the corresponding non-reacting flow. The anisotropy of Reynolds stresses and their dissipation rate tensors are found to be qualitatively similar. However, the components of the anisotropy tensors of Reynolds stress and viscous dissipation rate are not related according to a linear scaling, hence the models based on this assumption are not successful in capturing the viscous dissipation rate components obtained from the DNS data. By contrast, a model, which includes the invariants of the anisotropy tensor of Reynolds stresses and satisfies the limiting conditions for isotropy and 2-component limit captures the components of the viscous dissipation rate tensor more successfully for both non-reacting and reacting cases. Therefore, this model can be used for approximating the dissipation rate tensor in the Reynolds stress transport equation in the context of hybrid Reynolds Averaged Navier-Stokes/ Large Eddy Simulation modelling strategies.

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Impact of the Soret Effect on the Thermodiffusive Instability in Hydrogen Flames

Sofiane Al Kassar[1], Ollie Moore[1], William Lauder[1], Lukas Berger[2], Heinz Pitsch[2], Antonio Attili[1]

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Lean premixed hydrogen flames are prone to thermodiffusive instabilities, which originate from the differential diffusion between hydrogen and other species. The Soret effect, often called thermodiffusion, could play a role in augmenting differential diffusion due to thermal gradients. This study explores its impact on thermodiffusive instabilities in premixed flames at different pressure and temperatures, in both the linear and non-linear re-

gimes, via Direct Numerical Simulations with finite rate chemistry and detailed transport models. Various blends of hydrogen and methane are considered to discern the various effects.

In the linear phase, initially planar flames are exposed to weak multi-wavelength perturbations, allowing for the examination of growth rates for each harmonic. In the non-linear phase, a fully developed regime is achieved, and the characteristics of the complex and multiscale cellular structures emerging from the instability are analysed. In addition, the enhancement of the flame speed due to the instability is investigated.

The results reveal a gradual reduction in the influence of the Soret effect with increasing pressure and temperature. At ambient conditions, the Soret effect enhances differential diffusion effects, playing a significant role in the development of the thermodiffusive instability, while its impact is negligible at a pressure of 20 atmospheres.

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Analysis of thermodiffusive fluxes in hydrogen premixed flames using flamelet generated manifolds

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The development of reduced-order models is of paramount importance to reduce the computational cost associated with the chemical effects involved in reacting flow simulations. In particular, tabulated chemistry methods in the context of flamelet generated manifolds, have shown high potential to reproduce complex flow conditions from gaseous to spray flames with a high level of accuracy and reliability. In this study, an extension of this method to include detailed transport phenomena based on a mixture-average model is presented to describe the formation of thermodiffusive instabilities in hydrogen premixed flames. A dedicated analysis of the coupling terms involved in the thermodiffusive transport is performed and their weights across the flame front are examined to understand the contributions from each control variable to the global thermodiffusive balance. In addition, the modeling capability of the flamelet generated manifolds method is assessed with respect to the grid size and the strength of the thermodiffusive transport determined by the flow conditions.

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MS02-3 Direct numerical simulations, analysis, and modeling of premixed hydrogen flames (3)

Chair: Michael Gauding
Friday, May 10; 15:20 - 17:40; Room K

Data-driven modeling of thermo-diffusively unstable hydrogen-air flames

Pasquale Eduardo Lapenna[1], Arianna Remiddi[1], Francesco D'Alessio[1], Guido Troiani[2], Francesco Creta[1]

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State-of-the-art turbulent combustion models do not include the possible impact of thermo-diffusive instabilities, which have been shown theoretically, numerically, and experimentally to have a significant role in lean hydrogen premixed flames. In this contribution, we leverage variable fidelity data from both simulations and experiments to address the modeling of thermodiffusive unstable flames. The main idea is to develop a data-driven framework capable of reproducing the structure and propagation of unstable flames in both laminar and turbulent settings. This is done by resorting to the optimal estimator concept while using small- to medium-scale two-dimensional simulations of cellular hydrogen flames to generate tabulated thermochemical manifolds. Then the large eddy simulation (LES) sub-filter terms are closed using the Filtered-Tabulated-Chemistry-LES (FTACLES) formalism. The reference data are therefore filtered in the physical space and stored as a function of a properly defined set of filtered progress variables. A-priori and a-posteriori testing of the proposed framework is presented and discussed for laminar unstable flames. Then the inclusion of turbulent effects is discussed by means of the definition of a wrinkling factor term derived from both experiments and additional simulations. The modeling role of the synergistic interaction between turbulence and thermodiffusive instability is also discussed.

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Modelling of Turbulent Boundary Layer Flashback of a Lean Premixed Hydrogen Flame with Large Eddy Simulation and Flamelet Generated Manifolds Including Preferential Diffusion

Stijn Schepers, Rob Bastiaans, Roy Hermanns, Jeroen van Oijen
Eindhoven University of Technology, Netherlands

The high burning velocity and high diffusivity of hydrogen result in unwanted phenomena like flame flashback in combustion systems running on hydrogen. Especially in gas turbines, boundary layer flashback seems to be the prominent flashback mechanism, and accurate and efficient models are necessary to predict this unwanted phenomenon. In this research, a CFD combustion model is developed to investigate flame flashback in a turbulent boundary layer. The chemistry is reduced using the Flamelet Generated Manifold (FGM) method and extended to account for the large preferential diffusion effects of hydrogen. Turbulence is modeled using Large Eddy Simulation (LES), and the turbulence-chemistry interaction is modeled using a presumed beta probability density function (PDF). This FGM-LES tool is applied to a turbulent channel flow filled with a lean premixed hydrogen-air mixture. Initially, a cold flow simulation is performed to ensure a fully developed turbulent flow and the results are compared to DNS data reported in literature. Subsequently, a part of the domain is ignited to investigate flame propagation in the turbulent boundary layer. The FGM-LES tool is validated against DNS and experimental data of boundary layer flashback in similar turbulent channels reported in the literature. It is assessed if the preferential diffusion model in the FGM-LES tool captures thermodiffusive instabilities with sufficient accuracy and if the expected boundary separation zone is visible. Subsequently, the validated FGM-LES tool is used to study the influence of the wall temperature on the flashback behavior.

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Flamelet Generated Manifolds for lean premixed turbulent hydrogen flames

Gabriela Sanchez, Jeroen van Oijen
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The interest in developing models that can predict hydrogen combustion is continuously increasing. Hydrogen is a carbon-free alternative fuel; however, its high diffusivity leads to strong wrinkling of the flame and fluctuations of elements mass fractions and enthalpy along the flame front due to preferential diffusion. In this study, we investigate how the Flamelet Generated Manifold technique can be applied to model these phenomena. We performed Direct Numerical Simulations (DNS) of two cases with detailed chemistry and different Reynolds numbers. Then, we built several manifolds varying different parameters, such as equivalence ratio, temperature and heat release rate, in order to account for fluctuations caused by preferential diffusion. With these manifolds, we predicted species mass fractions and source terms, and we compared them to the DNS. For both cases, we found that two-dimensional manifolds with equivalence ratio fluctuations are sufficient to predict the main species mass fractions; however, it was necessary to add enthalpy as an independent variable to predict radicals mass fractions and source terms accurately. These results represent an advance in the development of a model for lean turbulent hydrogen combustion, further facilitating the execution of simulations of hydrogen flames in complex geometries such as gas turbines.

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Filtered tabulated chemistry for multi-regime hydrogen combustion

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Hydrogen represents a potential solution for the decarbonization of the aviation industry, however, new challenges arise due to transport and thermochemical properties which differ from conventional fuels. In practical applications, pure premixed injection is usually avoided to limit flashback propensity and both diffusion and partially-premixed flame structures, often stabilised by swirled injectors, are frequently observed in emerging burner designs. Multi-regime flamelet-type approaches for LES are popular due to their low cost, however, these approaches pose two key challenges: 1.) Correct distinction between combustion regimes and 2.) Coupling with the LES, where flame structures are unresolved at the mesh scale. The F-TACLES (Filtered tabulated chemistry for LES) model which couples tabulated chemistry with LES using the filtering approach, has been recently extended to account for multi-regime combustion by incorporating filtered 1-D partially-premixed flamelets. The distinction between combustion regimes is accounted for by the inclusion of the resolved scalar dissipation rate as a tabulation coordinate. This model is tested on the 3-D turbulent coaxial HYLON (Hydrogen Low-NOx) injector developed at IMFT in Toulouse. This configuration has two operating conditions, an attached flame (A) and a lifted partially-premixed flame (L). Both the attached and lifted partially-premixed

flames are investigated and compared against mono-archetype F-TACLES models.

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Manifold-based modeling for differential diffusion in turbulent premixed lean hydrogen flames

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Premixed lean hydrogen flames are subject to thermodiffusive instabilities induced by differential diffusion effects, and understanding and predicting differential diffusion and its effects on flame propagation and emissions are imperative for the widespread adoption of alternative hydrogen-based fuels. Manifold-based combustion models are attractive for reducing the computational cost of simulating turbulent reacting flows. While these models are often derived assuming unity effective Lewis numbers, one-dimensional manifold equations in progress variable for premixed combustion can be derived without such an assumption and are parameterized by the progress variable dissipation rate and curvature. This work will investigate how fluctuations in the progress variable dissipation rate and curvature influence both local and global flame behavior as well as manifold model performance. To study these phenomena, detailed simulations have been conducted for laminar and turbulent premixed lean hydrogen flames. The manifold model was evaluated both statistically and instantaneously against the simulation data. The results demonstrate how fluctuations in the progress variable dissipation rate and curvature influence flame structure and how each should be treated from a manifold modeling standpoint.

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Response of two-dimensional lean hydrogen-air laminar premixed flames to acoustic oscillations

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The response of two-dimensional lean hydrogen-air laminar premixed flames to acoustic oscillations has been analysed. Simulations for two equivalence ratios of 0.4 and 0.7 have been performed, to gain insights into the thermoacoustic response of lean hydrogen-air flames, which are prone to thermo-diffusive instabilities. The initially flat planar laminar flames have been subjected to acoustic oscillations representative of different sound pressure levels (SPL) to observe how acoustic waves influence the onset of flame wrinkling which triggers the thermo-diffusive effects induced by sub-unity Lewis number to further perturb the flame surface. It has been found that the flame response is sensitive to the strength of the imposed acoustic oscillation with different corrugation wavelengths observed on the flame surface for different sound pressure levels. The influence of equivalence ratio on the thermoacoustic response of the flames and the impact on the observed flame corrugations has also been assessed. Dispersion relations relating the perturbation growth rates to the flame surface corrugation wavelengths have been obtained and the effect of varying the frequency of imposed acoustic oscillation on the response of the flames has also been explored.

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Propagation characteristics of lean turbulent premixed ammonia-hydrogen flames

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Given the widespread interest in carbon neutrality, ammonia represents a potential energy carrier without carbon dioxide emissions. To obtain fundamental insights into the propagation and flame structural characteristics of fuel-lean turbulent premixed NH3-H2-N2-air flames in the presence of turbulence, three-dimensional direct numerical simulations are carried out with complex chemistry. In particular, we consider three mixtures with different levels of H2 ratio, specifically NH3-air, 60%NH3-25%H2-15%N2-air, and 40%NH3-45%H2-15%N2-air under fixed velocity and length ratios. To comprehensively assess the impact of diffusive-thermal imbalances on hydrogen-enriched ammonia flames, additional solutions with unity-Lewis-number transport were analyzed and compared with those obtained using the mixture-averaged transport model. The increase of H2 fraction in the fuel leads to elevated mean turbulent flame speed and stretch factor, indicating the impact of thermal-diffusive instability. The turbulent flame speed of the 60%NH3-25%H2-15%N2-air flame displays pronounced oscillations, a phenomenon absent in other mixtures considered in the current study. This behavior is attributed to the preferential diffusion of H2 mixed with the low-reactive NH3 in moderate quantities, resulting in a higher generation of flame elements extending into the product side and dynamic evolution of H2. The flame structure analysis, in terms of conditional averages, revealed a distinctive variation in H2 and H

atom distributions. The flames with a higher H2 fraction (40%NH3-45%H2-15%N2-air) produced a second peak of H2O2 in the trailing edge region, indicating additional production in the intense reaction zone. Additionally, in the 60%NH3-25%H2-15%N2-air flame, the reaction rate of H2 exhibited a unique behavior, with H2 being produced in the intermediate flame zone and rapidly consumed in the reaction zone, differing from other cases.

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MS03 Combustion Noise and Thermoacoustic Instabilities

Organizers: Abhishek Lakshman Pillai[1], Matthias Ihme[2], Ryoichi Kurose[1]

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MS03-1 Combustion Noise and Thermoacoustic Instabilities (1)

Chair: Abhishek Lakshman Pillai
Co-Chair: Matthias Ihme
Friday, May 10; 13:00 - 15:00; Room C

A Hybrid CFD/CAA Solver for Simulating Noise Generation in Real Fluid Flows under Transcritical and Supercritical Conditions

Abhishek Lakshman Pillai, Takuto Yamada, Sho Wada, Ryoichi Kurose
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Turbulent real fluid flows are encountered in the high-pressure combustors of supercritical gas turbine engines which offer the advantage of high thermal efficiency. However, reacting real fluid flows are also capable of generating significant noise whose mechanisms and characteristics remain to be fully understood. This work presents a hybrid CFD/CAA solver that considers real gas effects for simulating real fluid flows and describes the generation and radiation of noise from them. In this hybrid solver, Large-Eddy Simulation (LES) predicts the turbulent flow field, and the Linearized Euler Equations (LEE) are solved in the CAA simulation to predict the acoustic field. As a first step towards our future goal of applying the developed solver to simulate noise generation in transcritical and supercritical combustion, two inert nitrogen jets, one under transcritical (injected at cryogenic temperature) and the other under supercritical conditions, are simulated. Results show that the acoustic sources contributing to the low-frequency noise are located closer to the end of the jets' potential cores, while those contributing to the high-frequency noise are located further upstream. Furthermore, acoustic fields radiated by the transcritical jet and the supercritical jet are characterized in terms of noise directivity and spectral content of sound pressures.

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What is the potential of next-generation aviation gas turbine combustors for noise reduction?

Matthias Ihme[1], Davy Brouzet[1], Benyamin Krisna[1], Duane McCormick[2], C Aaron Reimann[2], Jeff Mendoza[2]
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Aircraft noise is a major concern because of its adverse effect on the quality of life, health, and property value of communities in proximity to airports and flight corridors. Recent progress in the development of advanced gas-turbine combustors offer opportunities to reduce noise emission. We present large-eddy simulations of a next-generation combustor and examine the emission of the direct and indirect combustion-noise contributions. To account for the complex geometry, a low-order acoustic reconstruction technique is developed that is based on a Green's function approach. Comparisons with a conventional rich-quench-lean combustor configuration show that that this advanced combustor concept has a direct effect on the acoustics, which is attributed to two specific technological novelties, namely (i) the reduced residence time due to compact combustor geometry and (ii) the reduction of the entropy inhomogeneities due the absence of dilution. These results provide opportunities for advanced combustion technologies to achieve substantial reductions in combustion noise.

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Numerical Analysis of Thermodiffusive Unstable Premixed Lean Hydrogen-Air Slit Flames

Borja Pedro Beltran, **Matthias Helmut Meinke**, Wolfgang Schroeder
RWTH Aachen University, Germany

Combustion noise appears in aero- and stationary gas turbines as well as in industrial boilers and furnaces. The acoustic modes generated by heat release fluctuations can interact with the gas filled plenum chambers or ducts

and lead to large amplitude low-frequency vibrations. These are generated by a dynamic feedback loop between the acoustic waves and velocity fluctuations causing flame front perturbations and thus heat release variations. Recently, hydrogen has received increasing attention as a renewable energy source. An important aspect in the development of hydrogen combustors, in which pure hydrogen or hydrogen-enriched natural gas are burnt, is the significant change in thermoacoustic stability.

In this work, lean premixed, two-dimensional hydrogen-air slit flames are investigated by using highly resolved numerical simulations. The fuel-air-equivalence ratio is varied and the impact on the general flame dynamics is investigated. For the various cases, intrinsic instabilities of the non-excited flame lead to strong cellular structures along the flame front, which cause constant pocket shedding and strong pressure fluctuations at the flame tip. Due to Markstein-length related effects, intrinsic differences are identified, when compared to methane-air premixed flames. A detailed investigation of the generated thermoacoustic modes is performed by solving the acoustic perturbation equations, in which acoustic sources determined from the flow field solution are used. These investigation enhance the understanding of the various acoustic source contributions to the overall acoustic field of premixed hydrogen-air flames.

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Exploring the connection between combustion noise and thermoacoustic instability

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Thermoacoustic instability, commonly initiated by combustion noise is one of the challenges hampering the development of cleaner gas turbines. This presentation will examine the link between combustion noise and thermoacoustic instability, using high-fidelity simulations such as direct numerical simulation (DNS) and large-eddy simulation (LES). The primary focus is on premixed flames, exploring the fundamentals of combustion noise, sound sources in premixed flames, and their contributions across the sound pressure level spectrum. The talk also examines the impact of hydrogen addition on sound generation in hydrogen/methane premixed flames, using results from our DNS studies. In the subsequent section, findings from LES of combustors fuelled with hydrogen/methane mixtures will be presented. The discussion will highlight the connection between combustion noise and thermoacoustic instability, underlining its implications for modeling. Finally, the presentation will offer insights into future directions for research, with a specific focus on enhancing our predictive capabilities for thermoacoustic instability.

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On the roles of spray response to pressure oscillations in combustion instability in a combustor with a lean-burn coaxially-staged fuel injector

Kazuaki Matsuura[1], Kodai Kato[1], Riko Hosoi[2], Yuta Sasaki[2], Yoshio Zama[2], Takeshi Yamamoto[1], Ryoichi Kurose[3]
[1]Japan Aerospace Exploration Agency, Japan, [2]Gunma University, Japan, [3]Kyoto University, Japan

Proper models on the fuel spray response to pressure oscillations driven by combustion instabilities are crucial to improve CFD. Fluctuation of fuel flow rate is especially significant as it induces equivalence ratio oscillation. However, such models do not seem to be fully established yet. In some literatures, a simple quasi-steady model was employed (Lieuwen and Zinn 1998 and Kato et al. 2008), whereas in others, the employed models were not explicitly described sometimes. On the other hand, Pillai et al. (2020) performed “numerical” experiments by LES on the effects of the artificially-introduced response delays, showing their notable impacts.

In our talk, two relevant attempts, still in progress, are to be presented.

Firstly, to investigate the impacts of the response, a similar approach to Pillai et al. was applied to a rectangular combustor equipped with a coaxially-staged lean burn injector. The results were compared with those similar to Matsuura et al. (2015). The injector with optical access into its pre-mixing duct provided information equivalent to fuel concentration, which can be used for fulfilling CFD validations.

Secondly, by means of a siren facility with a crossflow injection in a rectangular duct, the velocity inside its injection hole was measured by PIV to investigate the response. The aim was a new empirical model. It in fact showed deviation from the quasi-steady one. It was then introduced to the CFD above.

The numerical results on the quasi-steady response, the numerical experiments and the empirical model are to be presented and compared in our presentation.

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High-frequency transverse combustion instabilities of lean-premixed pure hydrogen-air flames

Kyutae Kim
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The present experimental investigation is concerned with combustion dynamics of lean-premixed pure hydrogen-air flames. To mitigate flashback risk in relatively fast premixed hydrogen flames, we use a multislit injector assembly with a slit width of 1.5 mm, of the same order of magnitude as the characteristic thickness of lean-premixed hydrogen flames. We carry out extensive measurements of self-excited pressure oscillations over a broad range of operating conditions between 30 and 100 kW thermal power. The experimental datasets are analyzed using the acoustic wave decomposition method, low-order thermoacoustic network modeling, and FEM-based three-dimensional Helmholtz simulations. We show that lean-premixed multislit hydrogen flames undergo strong high-frequency pressure oscillations between 3.1 and 3.5 kHz in excess of 25 kPa, originating from the triggering of the first tangential mode of the combustion chamber. We demonstrate that the transverse mode is characterized by high-amplitude spinning modes in the clockwise direction under relatively short combustor length conditions, discontinuously switching to counter-clockwise spinning modes at relatively long combustor length, and eventually transitioning to a moderate standing wave mode at the same resonant frequency. These observations demonstrate the previously unidentified complex modal dynamics induced by lean-premixed multislit hydrogen-air flames.

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MS03-2 Combustion Noise and Thermoacoustic Instabilities (2)

Chair: Abhishek Lakshman Pillai
Co-Chair: Matthias Ihme
Friday, May 10; 15:20 - 17:20; Room C

Modeling Considerations for Combustion Dynamics ROM Tools

Vishal Acharya
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Gas Turbine combustion systems operate in a variety of combustion paradigms ranging from premixed to gaseous diffusion to spray flames. In each of these cases, combustion instabilities occur with varying levels of propensity. During these instabilities, the unsteady heat release rate oscillations couples with one or more of the natural acoustic modes in a favorable feedback loop resulting in growth of pressure disturbances. These then lead to structural and thermal loads that are detrimental to the hardware, off-design operation leading to increased emissions and decreased efficiency and ultimately increased operating costs. To mitigate these instabilities, one design methodology uses robust acoustic network models of the gas turbine systems that incorporates the different volumes as acoustic elements with the heat release element comprising thermoacoustic coupling. This requires reduced order models for the heat release that can capture unsteady dynamics under different fluctuations for all the different operating modes. In this presentation, we shall cover system thermoacoustic modeling methodologies and specifically consider models for premixed flames, diffusion flames and spray flames that are suitable for a reduced order framework of a design tool.

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Numerical Analysis of Amplifying Longitudinal Combustion Instability in a Self-Excited Combustor

Seiji Tsutsumi[1], Noriyasu Omata[1], Taro Shimizu[1], Masahito Akamine[2], Junya Aono[3]
[1]Japan Aerospace Exploration Agency, Japan, [2]University of Tokyo, Japan, [3]Research Center of Computational Mechanics, Inc., Japan

A numerical study using compressible Large-Eddy Simulation with a flamelet progress variable approach was conducted to understand the self-excited longitudinal combustion instability in a Continuously Variable Resonant Combustor (CVRC) with an oxidizer inlet duct of 0.14 m. A numerical experiment in which the temperature of the inflow oxidizer was increased stepwise from 600 K in 20 K increments was conducted. The combustion noise with small amplitude was observed at 600 K. With the increase of the temperature, the self-exited combustion instability of the first longitudinal mode appeared, and this was remarkably amplified when the temperature changed from 700 K to 720 K. Using the phase-averaging method, vortex-driven combustion instability was observed in the case of 720 K. The period of the first longitudinal mode in the combustion chamber was almost equal to the sum of the period of the traveling wave in the oxidizer inlet duct and the time for the convection of vortex in the shear layer to the location of maximum heat release. In the case of 700 K, the timing of these phenomena was out of phase. The timing of these phenomena is essential for reduced-order models of combustion instability, and

a series of the authors' studies will be presented at this conference.

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Application of Matveev–Culick Model to Combustion Instability in a Self-Excited Combustor

Masahito Akamine[1], Seiji Tsutsumi[2], Taro Shimizu[2], Noriyasu Omata[2], Junya Aono[3]

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The reduced-order deterministic model for combustion instability involving vortex shedding proposed by Matveev and Culick (Combust. Sci. Tech. 175(6) 2003) and extended by Seshadri, Nair, and Sujith (Combust. Theor. Model. 20(3) 2016) is adapted to a single-element modeled rocket combustor called Continuously-Variable Resonance Combustor (CVRC) to understand the mechanisms of the self-excited longitudinal combustion instability and its transition dynamics. The original model is modified to represent (1) the sound propagation and reflection in the oxidizer inlet duct and (2) the interaction between the non-premixed flame and vortices, both of which have been identified as key elements of the feedback loop by a numerical simulation presented in the other part of authors' series of studies. The validity of the model is examined by comparing the results with the corresponding numerical simulations.

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Azimuthal instabilities in annular combustors

Nicholas Alexander Worth[1], Håkon Nygård[2], Abhijat Verma[2]

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Gas turbine engines are an integral part of the global energy production infrastructure. The ability to rapidly scale their power output makes them an attractive partner to intermittent renewable energy sources, meaning they are likely to retain their importance throughout the energy transition. However, designing future gas turbine systems that can operate in a fuel-flexible manner, accepting a wide variety of alternative carbon-free fuels is not straightforward, and hindered by our incomplete understanding of these fuels and some important phenomena which occur during their use, including combustion instabilities. In this talk recent experimental work on thermoacoustic instabilities in annular combustors will be presented, with an emphasis on the careful excitation of modes of interest, and the effects of realistic boundary conditions. Self-excited azimuthal modes in annular combustors can exhibit mode switching between spinning and standing states, and the orientation of the standing modes can change as a function of time. A multiple-input single-output azimuthal flame describing function is implemented into a quaternion valued low-order model to explore how different flame responses, caused by modes spinning in different directions, can affect the dominant mode of excitation.

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LES Study of Combustion Instability in a Laboratory-Scale Rocket Combustor

Shingo Matsuyama

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In the present study, large-eddy simulation (LES) is performed to simulate combustion instability in a laboratory-scale rocket combustor equipped with a single gaseous hydrogen/gaseous oxygen coaxial injector. LESs are conducted for corresponding combustion-instability experiments, and the self-excited combustion instability is successfully reproduced. The first tangential (1T) mode in the combustion chamber is captured by the LES, and its amplitude and frequency are consistent with the experimental observations. The coupling behavior between the flame motion and acoustic instability is investigated in detail from the LES results. The Rayleigh index calculated from LES flowfield data reveals that a driving factor for the instability is the unsteady pulsating-flame motion. The analysis of time series data indicates that the unsteady pulsating-flame behavior is caused by the coupling between the fuel injection and the 1T mode. The present study demonstrates the capability of LES to accurately capture the unsteady heat release and its coupling with pressure oscillations. LES is a powerful tool which can clarify details of flame structures that are not completely understood from the experimental measurements.

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Numerical investigation of thermoacoustic oscillation of a hydrogen micromix flame with LES

Daniel Kroniger[1], Hiromu Kamiya[1], Atsushi Horikawa[1], Ryuta Suzuki[2], Erik Munktell[3], Rene Braun[4]

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Numerical simulation of thermoacoustic instabilities in

a combustor is a promising method for modeling combustion induced thermoacoustic oscillations. The objective of this article is the analysis of instabilities of the hydrogen micromix flames. The micromix combustion principle has been developed for high hydrogen content fuels. This concept is based on miniaturizing non-premixed type flames to suppress NOx emissions. The risk of flashback is avoided by rapid mixing via jet-in-crossflow.

In this study, numerical simulations have been conducted with Simcenter STAR-CCM+ from Siemens Digital Industries Software. LES is used for turbulent modelling and resolving periodical phenomena. Two complete micromix flames with opposed injection direction are included in the computational domain. The boundary conditions are defined on the base of acoustic mode analysis results. The LES results are validated against experimental results from a test rig with generic micromix flame configuration. The solution of flow pattern is analyzed with POD for periodically recurring flow phenomena.

A strong periodical interaction of the flames at a thermal load of 170% (referred to the rated power of the gas turbine) could be found in the numerical results. The oscillation mode of the high-frequency regime is identified in the unsteady flow structure and confirmed via POD.

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MS04 Linearized Modelling of Flame Dynamics

Organizer : Thomas Ludwig Kaiser
Technical University Berlin

MS04 Linearized Modelling of Flame Dynamics

Chair: Thomas Ludwig Kaiser
Friday, May 10; 09:50 - 11:50; Room J

On the importance of turbulence modelling in a linear mean field analysis of turbulent flame configurations

Thomas Ludwig Kaiser[1], Thorsten Zirwes[2], Feichi Zhang[3], Kilian Oberleithner[1]
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Adjoint Linear Mean Field Analysis (LMFA) of turbulent reacting flows facilitates a holistic inverse design procedure with a focus on thermoacoustics and flame noise for real-world combustion systems. In laminar/stationary flames, the temporal mean state fulfills the non-linear governing equations of the flow, including the reaction model. Hence a linearization is possible, as demonstrated by various authors in recent years. LMFA of turbulent flames, however, poses a significantly more complicated challenge. Here, the temporal mean state does not fulfil the governing equations of the flow, introducing mean flow inconsistency issues during the linearization of the governing equations. We demonstrate that this problem can be circumvented by linearizing a Reynolds-Averaged Navier-Stokes (RANS) reaction model around the temporal mean state obtained by Large Eddy Simulations (LES). In the LES, the turbulent flame is acoustically actuated from the upstream direction by harmonic excitation. The analysis reveals that the linearized reaction model accurately reproduces the flame dynamics coherent with the harmonic actuation of an acoustically actuated turbulent Bunsen flame with high accuracy. However, it is also shown that state-of-the-art turbulence closure in the LMFA appears to inadequately describe the interaction of the background turbulence and the coherent flow fluctuation. Therefore, we investigate the interaction of turbulence and the coherent fluctuation using a priori and a posteriori analysis of different turbulence models. Furthermore, we discuss the necessity of introducing a new phase-averaging technique due to density variations, analogous to the Favre average in the RANS framework.

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Tri-Global stability analysis of reacting, swirling flows

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Swirling jets are used as canonical flow fields in combustion systems with the well-established advantage of a swirl-stabilized flame. The unsteady vortical hydrodynamic structures in these flows play integral roles in the operability and emissions of these combustors. However, modeling these structures and their impact on the flame remains challenging today. Hydrodynamic stability analysis has been a prominent and efficient technique for low order modeling of coherent structures for the past few decades. The objective of this study is to develop a reduced order model by the means of a Tri-Global hydrodynamic stability framework to gauge vortical flow modes of a swirling and reacting mean flow computed by Large Eddy Simulation based upon a commercial nozzle. Tri-Global linear stability analysis, which is often considered to be a computationally expensive technique in literature, is employed by exploiting the sparsity patterns of a linearized Navier Stokes equations through a high accuracy, centered finite difference scheme. Upon discretizing the linearized governing equations about a 7-point stencil, a generalized-eigenvalue problem is formulated leading to a sparse stiffness coefficient matrix. The GEVP is solved using a shift-and-invert technique to detect the natural, linear vortical modes of the base-flow in the global framework. A helical mode decomposition in carried out to extract the helical m modes commonly associated with swirling jets. Future work includes the addition of boundary forcing to simulate external noise and studying the harmonically forced global modes for the same base-flow.

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Identifying flame response mechanisms in a swirl-stabilised combustor using multi-layer networks

Vivek Thazhathattil, **Anindya Datta**, Saarthak Gupta, Santosh Hemchandra
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Thermoacoustic (TA) oscillation dynamics are investigated in the technically premixed PRECCINSTA swirl-stabilized combustor, for different methane-hydrogen fuel blends under atmospheric conditions using reacting flow large eddy simulation (LES). Prior work from our group analyzing the experimental data shows the presence of intermittent TA and precessing vortex core (PVC) oscillations for the pure methane case and coherent TA oscillations without a PVC with H2 enrichment. Multi-layer network analysis uses time series data from the LES solutions. We construct multi-layer networks connecting pressure at discrete points in the flow field with subnetworks for heat-release, mixture fraction and velocity fluctuations. Both inter-layer and intra-layer links are established based on information theoretic measures of causality (mutual information, transfer entropy), determined from the data within synchronized time windows. Time-varying weighted degree of connections between the heat release layer and other layers are expected to clarify the relative importance of velocity and mixture fraction fluctuations on TA and verify hypotheses made in prior studies. Additionally, we will use centrality metrics on velocity and mixture fraction layers to reveal the spatial positions of critical regions. Where meaningful, we will compare results from network analysis with those from physics-based stability and resolvent analysis to demonstrate the equivalence of both methods.

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Neural-network based Jacobians of non-linear closure terms for global linear analysis

Philipp Brokof, Axel Zimmermann, Wolfgang Polifke, Grégoire Varillon
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Global linear analysis of turbulent reactive flows promises sensitivity analysis and adjoint shape optimization of combustion systems, but relies on Reynolds triple decomposition that requires closure terms to model turbulence. While common two-equation closures for turbulent stresses and heat release rate in the Reynolds averaged Navier Stokes (RANS) equations can be linearised directly, their accuracy is often insufficient compared to large eddy simulations (LES) that are state of the art for reactive flows. As a remedy, the assimilation of case-specific RANS closures that reproduce LES mean fields with physics informed neural network has been proposed. However, upon finding such a closure, the question arises how to incorporate it in a global linear analysis. Here, we suggest a purely data driven approach, encoding the local non-linear mapping from the flow's state vector to the closure in a second neural network (NN), and subsequently exploiting the NN's direct differentiability to obtain the Jacobian of the closure needed for linear analysis. We explore the feasibility of the idea on increasingly complex cases, for which the non-linear closure is known, by comparing linear transfer functions obtained from NN-based Jacobians with those obtained from the non-linear equations under small forcing.

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Subcritical bifurcation of a premixed annular V-flame

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This work aims to characterize the self-excited axisymmetric oscillations of a premixed laminar V-flame, in an annular jet of lean premixed methane and air. The flame is anchored near the rim of the centerbody, forming an inverted cone, whereas the strongest vorticity is concentrated along the outer shear layer of the annular jet. Consequently, the reaction and vorticity dynamics are largely separated, except near the flame tip, where both coalesce. The global eigenmodes corresponding to the linearized reacting flow equations around the steady base state are computed in an axisymmetric setting. We identify an arc branch of eigenmodes exhibiting strong oscillations at the flame extinction. Unlike the other categories of eigenmodes present in the eigenspectrum, the eigenvalues associated with the arc branch are unaffected by the domain size and become destabilized as the Reynolds number increases. The frequency of the leading eigenmode is found to be nearly identical to the Lagrangian advection time from the nozzle outlet to the flame surface along the inner shear layer. This linear result suggests a non-local intrinsic feedback mechanism involving interactions between perturbations at the nozzle edge and the flame tip. Nonlinear time-domain analysis also reveals this instability to be subcritical. Hence, even when the flame is linearly stable, perturbations of sufficient amplitude can trigger limit-cycle oscillations sustained by nonlinear feedback.

Notably, linear analysis of the time-averaged limit-cycle state yields eigenmodes that do not match the nonlinear oscillation frequencies, due to the system's strong nonlinearity.

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MS05 Liquid Ammonia Spray and Combustion: Numerical Modelling

Organizers: Jiangkuan Xing[1], Christine Rousselle[2]

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MS05-1 Liquid Ammonia Spray and Combustion: Numerical Modelling (1)

Chair: Jiangkuan Xing
Co-Chair: Christine Rousselle
Friday, May 10; 13:00 - 15:00; Room B

High-fidelity modelling of liquid ammonia spray and combustion

Jiangkuan Xing, Zhenhua An, Ryoichi Kurose
Kyoto University, Japan

Directly using liquid ammonia can simplify the fuel supply system and reduce the start-up time. Liquid ammonia will undergo flash boiling with strong heat loss due to its low boiling point and is usually co-fired with small-molecular fuels for better stabilization. How to accurately model the unique phase change and the subsequent combustion processes is still an open question. To this end, this study aims to establish high-fidelity and efficient modeling strategies for liquid ammonia spray and combustion. Specifically, a combined phase change model is developed for describing the ammonia flash spray, and its accuracy and superiority are assessed under various conditions by comparing the predictions with the experimental data and other models' predictions. Subsequently, liquid ammonia combustion in a temporally evolving mixing layer is studied using direct numerical simulation (DNS) with detailed chemistry to provide a deep insight into the multiple fuel streams and strong heat loss. Extended flamelet-based models are developed considering the complicated fuel streams and strong heat loss. Their performances are evaluated with the DNS data as benchmarks. The premixed mode dominates in the liquid ammonia combustion, and the premixed flamelets are recommended to be used for the liquid ammonia flame.

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Computational singular perturbation analysis applied to evaporation of ammonia droplets

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Computational singular perturbation (CSP) has been effective in analyzing complex chemically reacting flows by systematically retrieving intrinsic timescales and slow invariant manifolds. This study marks the inaugural application of the analytical and computational framework to scrutinize Lagrangian droplets experiencing evaporation and dispersion in the adjacent gases. The mathematical formulation is derived to integrate CSP tools into the droplet dynamics equations, with the tangential stretching rate (TSR) to characterize the explosive/dissipative nature of the system. Ammonia droplet case studies are subsequently conducted. The CSP indices indices are explored to offer a comprehensive analysis of different subprocesses and their interplay in modifying droplet dynamics and justify the roles of mass-driven and thermally-driven regime evaporation regimes at different environmental temperature.

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Observation of liquid ammonia spray structure injected from a pressure-swirl nozzle up to elevated pressure

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To clarify liquid ammonia spray characteristics are important for development of ammonia-fueled gas turbine.

In addition, detail understandings of liquid ammonia spray are important for the modeling of numerical simulation. In this study, the structure of liquid ammonia spray injected from a pressure-swirl nozzle up to elevated pressure were experimentally investigated. Experiments were performed for non-reacting flows using a high-pressure chamber, and the environment pressure increased up to 0.7 MPa. The liquid ammonia spray structure was observed using high-speed backlight imaging. The structure of liquid ammonia spray was compared with that of ethanol spray structure to clarify the effects on flush boiling on spray formation characteristics. Also, the liquid ammonia spray was characterized using the degree of superheat. The high-speed backlight images showed that the the spray angle of liquid ammonia spray increased with an increase in the environmental pressure. For the liquid ammonia temperature of 294 K, the spray density seems to be changed non-monotonically with an increase in the pressure. In this study, to clarify the liquid ammonia spray characteristics in detail, laser diagnostics were employed.

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Numerical study of the flame structure and interaction between droplet/flame of LNH3 spray flame in a swirl combustor

Jiawen Liu[1], Meng Zhang[1], Zhenhua An[2], Jinhua Wang[1], Zuohua Huang[1]
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Direct combustion of liquid ammonia has the potential to reduce system costs and heat loss of gas turbine (GT). However, its tendency to flash and the high latent heat of vaporization can lead to combustion deterioration. Previous research suggests that stabilizing a liquid ammonia flame requires swirl and preheated air. So far, the specific flame structure and interaction between the spray and flame of a liquid ammonia swirl flame remain inadequately explored. To fill this research gap, the liquid ammonia spray model was first validated based on particle drop image analysis and thermocouple temperature measurements. Subsequently, utilizing the OpenFOAM-8 platform, a detailed investigation of the flame and spray behaviors in a swirl burner using pure liquid ammonia as fuel was carried out through a large eddy simulation. The findings revealed that the droplet evaporation time scale is notably shorter than the convection time scale, resulting in nearly no single droplet combustion regime occurring in the present configuration. The rapid evaporation of droplets generates a preheating zone with a distinct temperature and NH3 concentration gradient between the flame and the spray area for preheating the fresh mixture. The flame exhibits the characteristics of a pre-evaporated gaseous flame, which shows a complex, mainly non-premixed structure, yielding various combustion modes. Furthermore, the flame base exhibits noticeable heat loss, which leads to frequently observed local extinction phenomena. This is primarily caused by the increase of the evaporation source term, while the increase of scalar dissipation rate shows minimal effects.

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Direct numerical simulations of combustion characteristics with liquid ammonia direct injection under engine-like conditions

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Ammonia is an ideal zero-carbon fuel and it can be used directly in a liquid state. However, the utilization of liquid ammonia in engines is constrained by its unique physical and chemical properties. Direct injection of liquid ammonia is a promising solution for internal combustion engines, but its combustion characteristics are not well understood yet. In the present work, liquid ammonia direct injection under compression ignition engine-like conditions is investigated using direct numerical simulation (DNS) and the combustion characteristics of ammonia spray are analyzed. The ammonia spray is injected from a circular nozzle, where the ammonia spray is auto-ignited under engine-relevant thermochemical conditions, resulting in complex turbulent ammonia spray combustion. A low Mach number DNS code is employed for solving the conservation equations for reacting flows with detailed chemistry, in which block-structured adaptive mesh refinement is implemented to reduce the computational cost. Using the DNS data, the ignition and combustion processes of the ammonia spray are analyzed. The emission characteristics of the ammonia spray flame are examined. The interactions between the turbulence and ammonia spray jet flame are also reported.

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Liquid ammonia spray : flash-boiling phenomenon

Christine Rousselle, Camille Hespel
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Ammonia is a very interesting alternative for thermal applications as gas turbines and internal combustion engines. The injection of liquid ammonia into the combustion chamber has the double advantage of doing away

with a vaporization system and stratifying the local air/fuel mixture during combustion. Ammonia has a very high saturation vapor pressure compared to other e-fuels such as methanol. Therefore, during the expansion within the injector, bubbles can be created and generate atomization and vaporization described as flash boiling phenomena, accompanied by a strong cooling of the medium due to its high latent heat of vaporization. The objective will be to provide a review of the recent experimental data which provide further analysis of the process, to highlight the scientific questions and last to question about the challenges to model it for accurate simulations.

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MS05-2 Liquid Ammonia Spray and Combustion: Numerical Modelling (2)

Chair: Jiangkuan Xing
Co-Chair: Christine Rousselle
Friday, May 10; 15:20 - 17:00; Room B

Models for liquid ammonia sprays: developments on Eulerian and Lagrangian approaches

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Predictive models for liquid ammonia sprays are of utmost importance for the development and optimization of direct injection engines and gas turbine burners. This work presents developments for both Lagrangian discrete parcel method, and Eulerian multiphase approach. Ammonia poses new challenges because of its high latent heat of vaporization and the low vapor pressure which easily induces flash boiling, externally or also internally in the nozzle.

Within the Lagrangian method, a correlation for the primary breakup is proposed to determine droplet sizes and near-exit jet cone angle, to reproduce seamlessly flash-boiling and non-flashing regimes. Also, a model based on nucleation and growth of bubbles within liquid droplets is discussed, whose main feature is the prediction of a radial momentum transfer resulting from droplet explosions.

The Eulerian model, capable of resolving the internal and external nozzle flow, uses a flash-boiling mass transfer model adapted to ammonia properties and is based on single-fluid formulation, also referred to as four equation model. A drift-flux model version is presented which includes a velocity slip model.

Reynolds Averaged Navier Stokes (RANS) approach for turbulence is used. Numerical results for each approach are compared with experimental liquid and vapor tip penetrations, spray morphology and Sauter Mean Diameter (SMD) measurements, for a multi-hole and a single hole injector. In addition, local temperature predictions are discussed, for both liquid and gaseous phases, highlighting and quantifying the strong cooling effect that ammonia produces during the phase change process.

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Numerical investigation of flash-boiling atomization characteristics of liquid-ammonia fuel at various superheat degrees

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Recent studies on gaseous ammonia combustion have shown that ammonia will be an important energy vector in a carbon-neutral society by 2050. World-first 50 kw gaseous ammonia gas turbine systems was built in Fukushima, Japan. However, ammonia is commercially available as a liquid in high-pressure cylinders at room temperature. Thus, it has been reported that considerable energy is consumed by vaporizer and compressor when liquid ammonia is converted to gaseous ammonia. On the other hand, high pressure is an exceedingly important factor in improving the efficiency of gas turbine systems in terms of thermodynamics. Therefore, the ammonia gas turbine using liquid ammonia spray combustion contributes to improving the efficiency of the entire gas turbine system including peripheral equipment.

Recent numerical and experimental studies on liquid ammonia spray characteristics and combustion showed that releasing high-pressure liquid ammonia through a nozzle below the saturation pressure causes the liquid to be superheated, resulting in-tense flash boiling. On the other hand, flash-boiling spray characteristics such as plume angle, droplet size, penetration distance are highly dependent on superheat degree and nozzle geometries and surface roughness. Thus, in this study single hole nozzle injector was used to visualize the spray patterns using backlight images and the degree of super heat is varied by altering combustor ambient pressure and liquid ammonia injection temperature. The bubble nucleation density, bubble departure frequency, and vapor volume fractions were calculated numerically using a nucleation theory. The droplet diameter reduction factor of liquid ammonia at various superheat degrees was numerically obtained and compared with alcohol and alkane liquid fuels.

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Internal and Near-Nozzle Flow of Ammonia Using the ECN Spray G Injector

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The global transportation sector is undergoing a shift from fossil-based fuels to carbon-free alternatives due to the adverse effects of burning fossil fuels on climate, health, and limited resources. Ammonia is a promising carbon-free fuel due to its relatively simple synthesis from green hydrogen and its superior storage capabilities when compared to pure hydrogen. However, challenges persist, with limited understanding of ammonia combustion and spray behavior during high-pressure injection. This research focuses on the near-nozzle spray behavior during direct injection of ammonia. Computational fluid dynamics simulations of flash-boiling ammonia injection through the Engine Combustion Network's Spray G 8-hole fuel injector were performed. An in-house solver that accounts for thermal non-equilibrium using the Homogeneous Relaxation Model (HRM) was used. The simulations were carried out at varying injection temperatures and ambient pressures and compared with each other. Shock structures in the spray due to supersonic flow velocities were found to be present at injections with a degree of superheat as low as Rp = 8.5, causing the spray to collapse, increasing spray penetration and threatening wall wetting. The high rate of vaporization combined with ammonia's high enthalpy of vaporization results in a severe temperature drop in the combustion chamber, possibly impacting steady and efficient combustion.

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Numerical investigation of liquid ammonia combustion in MILD conditions

Zhenhua An, Jiangkuan Xing, Ryoichi Kurose
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Abstract: Liquid ammonia has received increasing attention as a carbon-free fuel in power equipment due to its advantage in simplifying the system and shortening the start-up time. However, low combustion intensity and high NOx emissions pose challenges for liquid ammonia combustion applications. Moderate or Intense Low oxygen Dilution (MILD) combustion technology is a promising approach to enhance the combustion stability while keeping the NOx emissions at an acceptable level. The present study aims to numerically investigate the ammonia spray flames under MILD conditions. Specifically, series of temporally evolving ammonia spray jet flames, stabilized in a hot co-flow, are investigated using detailed chemistry. Different co-flow conditions (oxygen concentration and temperature) are considered, including the MILD combustion, high temperature combustion (HTC), and traditional combustion (TC) conditions. The detailed chemistry and diffusion are considered in the numerical method. The combustion stability and emission performance under MILD conditions are explored and compared with those under the HTC and TC conditions to highlight the differences.

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Numerical investigation of hydrogen-fired prechamber ignition of the ammonia main charge in reciprocating engines

Thomas Indlekofer, **Nils Erland L. Haugen**, Andrea Gruber
SINTEF Energy Research, Norway

Ammonia-fired reciprocating engines have emerged as a promising technology in the maritime and power-generation sector at medium scale (1-10 MW). The use of ammonia cracking to produce small quantities of hydrogen that can be used as a combustion promoter instead of fossil fuels, enables this technology to provide a purely carbon-free propulsion and power-generation technology. In this context, a hydrogen-fired prechamber turbulent jet ignition approach has been proposed and it is envisioned to offer significant advantages by accelerating the ammonia ignition and combustion process, increasing its reliability and completeness and achieving low NOx, N2O and NH3 emissions if combined with a non-premixed ammonia flame configuration. This study exploits an OpenFOAM-based Large Eddy Simulation (LES) model to investigate the combustion behaviour of an ammonia main charge ignited by a hydrogen-fired prechamber. Firstly, a conventional port-injection configuration for the ammonia main charge is considered and the hydrogen-fired prechamber is found to provide a strong ignition source for ammonia-air mixtures. The effect of the main-charge equivalence ratio and of the wall temperature on combustion efficiency and emissions formation is evaluated. Secondly, the same hydrogen-fired prechamber configuration is shown to be able to successfully ignite a liquid ammonia main charge directly injected as a spray and modelled using Lagrangian Point Particles (LPP).

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MS06 Detonations in Liquid-Fuel Sprays: Recent Progress and Open Questions

Organizers: Alexei Poludnenko[1], Hai Wang[2]

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MS06-1 Detonations in Liquid-Fuel Sprays: Recent Progress and Open Questions (1)

Chair: Alexei Poludnenko
Co-Chair: Hai Wang
Wednesday, May 8; 10:40 - 12:20; Room I

Numerical Modeling of Gaseous and Spray Detonations in Hydrocarbon Fuels using Complex Chemistry

Alexei Poludnenko, Sai Sandeep Dammati, Abeetath Ghosh
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Recent years have seen a resurgence of interest in detonation-based propulsion systems. Design and development of such systems requires accurate and predictive numerical modeling of detonations both in gaseous and liquid hydrocarbon fuels. This in turn relies heavily on the fidelity of the underlying physical and chemical models, including the description of chemical kinetics, as well as spray droplet drag, evaporation, and secondary atomization. Most of these constituent models have been developed for low-speed combustion and multi-phase flow regimes, and their accuracy and applicability in the extreme flow conditions characterstic of detonations is not clear. In this work, we use two- and three-dimensional Eulerian-Lagrangian simulations of spray detonations propagating in liquid n-dodecane to perform the detailed characterization of the hydro- and thermodynamic regimes experienced by the spray in a detonation front. These calculations use complex chemistry, multi-species transport, and state-of-the-art spray sub models. Furthermore, we compare the observed dynamics and properties of spray detonations with their purely gas-phase counterparts both in the pre-vaporized n-dodecane, as well as in other gaseous hydrocarbon fuels. Finally, we discuss the applicability of the existing spray sub-models and their required extensions for the accurate modeling of spray detonations.

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A molecular view of shocks and shock-droplet interactions

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Gas-phase and two-phase detonations are characterized by small spatial regions of thermodynamic nonequilibrium, which may impact mass, momentum, energy transport, and chemical reactions in a manner that is not suitably described by the Navier-Stokes equations and conventional chemical kinetics. To examine these effects, we carried out a series of molecular dynamics (MD) studies targeting a better understanding of several phenomena with direct relevance to gas-phase and spray detonations. These problems include translational nonequilibrium in shock fronts, vorticity generation near triple points, shock-induced transport of long-chain molecules behind the shock, shock-droplet interactions, and the resulting droplet fragmentation upon shock impact. The focus of the analysis is on the effect of non-equilibrium on the transport of mass, momentum, and energy behind a shock front. The implications of the findings on detonation physics, chemistry, and simulations will be discussed in detail.

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Detonation propagation in droplet-laden flows

Venkat Raman, Ral Bielawski
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Multiphase detonations pose a number of modeling and computational challenges. This includes, but not limited to, the description of shock-induced breakup of droplets, propagation of shock-reaction fronts through dense spray medium, evaporation and inhomogeneous mixing of fuel with oxidizer, and the initiation of reactions in these highly complex and time-varying fields. In this talk, preliminary findings on the shock-droplet interactions, and extensions to reaction coupling in dense spray regime will

be discussed. Where applicable, comparisons with experiments will be shown. A summary of the critical modeling and data needs will be provided.

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Numerical Study on the Effect of Droplet Spatial Distribution on Liquid-Fueled Detonation

Manoj Paudel, Jacob McFarland
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This study investigates the impact of initial droplet spatial distribution, in particular the presence of droplet clusters, on the multiphase detonation phenomena. 2D Euler-Lagrange simulations with low vapor pressure liquid fuel (n-decane) and air(N2/O2) will be presented. The hydrodynamic code FLASH is used for the solution of reactive Euler equations with multiphase source terms where coupling is achieved through operator splitting. The directionally split Piecewise Parabolic Method (PPM) and Bader-Deuflhard method implemented in FLASH will be used for the solution of Euler equations and the system of ODEs from reaction kinetics respectively. Interchange of variables and source terms from particles to gas (and vice versa) is achieved with bi-linear mapping of variables between the Lagrangian points and Eulerian mesh. A three step reduced mechanism tuned to reproduce ZND parameters of the detailed mechanism for variable equivalence ratios is used for reactions in the gas phase. For the particle phase, deformation, evaporation and breakup will be considered through the modified Taylor Analogy Breakup (TAB) model, Abramzon-Sirignano evaporation model, and Kelvin-Helmholtz Rayleigh-Taylor (KHRT) breakup model respectively. Simulations for both globally lean and rich mixtures with varying degree of initial clustering of micron sized droplets will be presented to study the detonation speed and structure under heterogeneous multiphase conditions.

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Wedge-stabilized oblique detonation in n-dodecane droplet and air mixtures

Huangwei Zhang
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This study numerically investigates wedge-induced oblique detonation waves (ODW) in n-dodecane droplet/air mixtures under real flight conditions. The results reveal that the discrete droplets introduce considerable non-uniformity and unsteadiness in the ODW. Specifically, the 5-μm droplets can complete evaporation slightly after the oblique shock wave, resulting in an increased initiation length compared to the gaseous ODW with the same equivalence ratio. The deflagration front is irregular and peninsula shaped. The transition mode exhibits a combined smooth and abrupt modes. The effects of droplet size and flight altitude on the ODW morphology are also studied. As the droplet diameter increases, there is a corresponding increase in droplet penetration distance in the induction zone, shifting the evaporation front downstream. The angle of the oblique shock wave slightly increases, and the reaction front changes non-monotonically as the droplet size varies. Moreover, with increasing flight altitude, the significant decrease in inflow pressure leads to reduced droplet evaporation rate and therefore increased droplet penetration distance. The results also show that the transition mode is significantly affected by the droplet size and flight altitude.

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MS06-2 Detonations in Liquid-Fuel Sprays: Recent Progress and Open Questions (2)

Chair: Alexei Poludnenko
Co-Chair: Hai Wang
Wednesday, May 8; 13:30 - 15:10; Room I

Molecular hotspots and shock enhanced transport in detonation waves

Matei Radulescu, Ramki Murugesan
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Detonation waves in gases and multi-phase systems are very complex, involving a highly transient cellular structure and a turbulent reaction zone coupled with transverse shocks. The role of out-of-equilibrium phenomena in these waves remains unclear despite extensive research on the underlying physics. Using hard sphere molecular dynamics simulations for a single activated exothermic reaction, we demonstrate and quantify two fundamental mechanisms where species resulting from a reactive collision provide modification of the surrounding reactivity and wave sustenance. First, we demonstrate the role of molecular hotspots, first predicted by Prigogine. Species evolving from a reactive collision have a substantial excess of translational energy. This excess energy serves in promoting neighboring reactive collisions. The absence of molecular chaos accelerates the reactivity by a factor of two (Murugesan et al. Comb. Flame 2019). The role of out-equilibrium reactions is

further demonstrated in the presence of shock waves by a mechanism first postulated by Zel'dovich (Murugesan PhD 2023). We study the problem of shock to detonation transition using molecular dynamics of a single exothermic reaction. Results suggest that shock-induced ignition and transition to detonation involve non-equilibrium reactions that overlap with the shock structure, showing strong translational non-equilibrium with reactive fingers. We find that shock amplification rate and transition to detonation are approximately twice faster than predicted by conventional continuum Euler hydrodynamic models. A Navier-Stokes model with hard sphere transport properties effectively captures the acceleration process.

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Pathological propagation regimes in liquid-fuel detonations

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Detonation waves are supersonic reactive fronts involving strong pressure variations, which propagate in a self-sustained manner when a sonic surface isolates them from downstream conditions. In ideal gaseous detonations, it is possible to predict the Chapman-Jouguet velocity associated with the sonic condition based on equilibrium states.

Nonetheless, there exists a distinct propagation regime called pathological detonation, wherein the sonic condition is not attained at the equilibrium state but within the reactive region. This regime may arise when endothermic effects are considered, leading to the formation of an internal sonic point where local thermicity vanishes. The self-sustained propagation regime is then obtained placing the sonic point in the neutrally thermal zone, which requires studying the detonation structure. Indeed, endothermic effects acting behind the sonic point are decoupled from the detonation propagation mechanism, leading to higher propagation speeds. This regime is commonly analyzed for endothermic and exothermic competing reactions of multistep chemical schemes. However, this study extends the understanding of pathological detonations, revealing their occurrence in liquid-fueled detonations where droplet vaporization dominates the late stage of the non-equilibrium region. The range of appearance of such detonations is shown to increase with the fuel droplets Stokes number and the mixture equivalence ratio.

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The Influence of non-premixed heat combustion on spray detonations

Ryan Houim

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Numerical simulation of stoichiometric JP10 and air detonations were performed. The governing equations representing a fully compressible reactive gas and an Eulerian model to represent the JP-10 droplets were solved. The results show a cellular multiphase detonation consistent with previous literature. Two heat release zones were found. A primary heat release occurs in a narrow region (~5-10 mm) behind the leading shock where the droplets are convectively heated, vaporize, and burn in the shock-heated air. A secondary heat release occurs over an extended region where fuel-rich pockets continue to burn as turbulent non-premixed flames. The secondary non-premixed heat release zone is caused by multiphase flow effects that occur in the primary heat release zone.

Finite Stokes number effects cause the droplets to lag behind the shock wave while the air is compressed immediately. Droplet inertia effect produces a thin band where the local equivalence ratio decreases substantially. Eventually, the droplets accelerate in the post-shock flow and the local equivalence ratio increases and even becomes fuel-rich in small regions. This results in alternating fuel-rich and fuel-lean regions that persist throughout the primary reaction zone and continue to burn in the secondary heat release zone as non-premixed flames. This secondary non-premixed heat release zone is unique to sprays and its influence on the detonation structure is not well understood.

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Nonthermal termolecular reaction effects on planar and oblique detonations

Jacqueline H Chen[1], Akanksha Baranwal[2], Jorge Salinas[1], Swapnil Desai[3], Yujie Tao[4], Ragu Sivaramakrishnan[5]

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In applications involving fast transport conditions including supersonic transport and planar and oblique detonations, there is a high probability of occurrence of non-thermal reactions due to the presence of non-trivial amounts of highly reactive radicals including H, O and OH apart from O2 as demonstrated recently (M. P. Burke et al., (2017), Tao et al., (2021)) that participate in collisional cooling. High-fidelity simulations were performed to assess the significance of non-thermal reactivity induced by radical-molecule association and radical-radical recombi-

nation reactions on the initiation, propagation and structure of planar and oblique detonation waves for different mixture conditions. It is found that non-thermal reactivity induced by radical-molecular association reaction R5: H+O2 (+M) ↔ HO2 (+M) and radical-radical recombination reaction R16: H+OH (+M) ↔ H2O (+M) can alter the wedge-stabilized oblique detonation wave (ODW) and planar detonation wave (PDW) propagation and structure.

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Numerical modeling of chemical combustion induced by blast waves interactions

Fumiya Togashi[1], Joseph D Baum[1], Rainald Lohner[2], Orlando A Soto[3], Mariana Cruz[4]

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Combustion of spatially dispersed liquid chemical upon interaction with a blast wave was investigated in this effort. The numerical simulation modeled a test in which a plastic bottle filled with the liquid simulant and a small explosive detonator were hung in a chamber, while a primary explosive charge was hung some distance away. The primary charge detonation was delayed to allow evolution of the spray prior to interaction with the blast environment The oxygen balance in the chamber was positive.

A CFD methodology capable of modeling the complete set of physical processes was required to better understand the controlling physical mechanisms. Explosive detonation was modeled using the Jones-Wilkins-Lee (JWL) equation of state, while simulant reaction was modeled using Chemkin-II, coupled with our in-house CFD solver. A reduced kinetics reaction model based on the GRI-Mech3.0 combined with simulant decomposition kinetics was developed. The numerical model incorporates a volume-of-fluid methodology. Turbulence was modeled using a MILES (Monotonically integrated LES) model. The most challenging part was the accurate modeling of the liquid bulk break-up to ligaments and further to large droplets, as no theoretical or even an empirical model exists for this phenomenon. A 0-D analysis of simulant droplet heat transfer and ignition was also conducted prior to the full-scale simulation. The analysis indicated the importance of the numerical modeling of liquid aerosolization during the dispersion and cascading into small droplets by the blast wave interaction.

The numerically predicted bottle break and liquid dispersion agreed well with the test visualization data, and the predicted pressure captured the pressure changes during evaporation and reaction. The excellent agreement of the measured and predicted pressure histories indicates that the current numerical methodology accurately models simulant combustion as well as all other controlling physical mechanisms.

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MS06-3 Detonations in Liquid-Fuel Sprays: Recent Progress and Open Questions (3)

Chair: Alexei Poludnenko
Co-Chair: Hai Wang
Wednesday, May 8; 15:30 - 17:10; Room I

Modeling of High-Pressure Transcritical Phase Change at Liquid-Fueled Detonation Conditions

Navneeth Srinivasan, Suo Yang
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Liquid-fueled detonation engines are of significant interest due to the on-board practicality of storing liquid fuels comparing to gaseous fuels. With pressures of 20-40 bar or higher, these engines involve thermodynamically transcritical and supercritical processes, such as evaporation facilitated by transcritical shock/detonation interaction and high-temperature mixing. Fuel-air mixtures are multi-component, complicating matters with elevated mixture critical points compared to individual constituents. This necessitates thermodynamic modeling to understand liquid fuel interactions with detonation waves, thickened interfaces, weakened surface tension, and transcritical phase change. The vapor-liquid equilibrium (VLE) theory, a first-principled model describing multiphase thermodynamics, faces computational challenges and robustness issues when integrated with CFD modeling. Ongoing efforts address these challenges, including developing reduced-order models, shared-memory in-situ adaptive tabulation (ISAT) of VLE solutions, and an artificial neural network (ANN)-aided VLE model. These approaches have been applied to study transcritical shock-droplet interactions and (reacting) turbulent mixing layers, offering insights into transcritical fluid behavior. Questions persist regarding fuel droplet evaporation at elevated pressures. Primary tests on droplet evaporation using the ANN-aided VLE model reveal a potential decrease in evaporation timescales near critical points. Additionally, exploring non-equilibrium droplet physics remains an open question, emphasizing the importance of understanding equilibrium solutions for model development, even in non-equilibrium scenarios.

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Vibrational Nonequilibrium Effects in Hydrogen Detonations

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Detonations in gaseous systems exhibit vibrational nonequilibrium not only through the induction zone but also throughout the reaction zone, potentially affecting both hydrodynamic and chemical reaction characteristics. In general, reactant species are vibrationally cold and translationally hot, resulting in competing effects that simultaneously suppress and enhance reaction rates, respectively. This imbalance of energy modes can even persist into the post-reaction product state. Due to the chaotic nature of gaseous detonations, it is not clear that these competing effects will simply cancel out, particularly in unstable detonation regimes. We seek to further assess these nonequilibrium processes and their physical effects in gaseous, hydrogen-based detonations. To this end, we will present a vibrationally-informed equation of state and reaction rate model that accounts for energy exchange between translational-rotational, vibrational, and chemical modes. A multi-temperature approach will be implemented, which leverages a common translational-rotational temperature and a set of species-specific vibrational temperatures. This model will be utilized to numerically assess how different ambient conditions, such as varied inert species at varied concentrations, affect the induction and reaction zones as well as detonation stability (pulsation) characteristics.

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MS07 Computational Tools for Detonation-Driven Propulsion Physics

Organizers: Jiro Kasahara[1], Venkat Raman[2], Jeong-Yeol Choi[3], Akiko Matsuo[4], Nobuyuki Tsuboi[5]

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MS07-1 Computational Tools for Detonation-Driven Propulsion Physics (1)

Chair: Jiro Kasahara
Co-Chair: Akiko Matsuo
Friday, May 10; 09:50 - 11:50; Room G

Numerical Analysis of the Characteristic Chemical Time-scale in a C2H4/O2 Non-premixed Rotating Detonation Engine

Jeong-Yeol Choi, **Mohammedniyasdeen Nejaamtheen**
Pusan National University, Korea

This study elucidates the characteristic chemical kinetics timescales pertinent to rotating detonation engines (RDEs). The presence of supersonic-speed detonations in an RDE gives rise to a highly intricate reacting flow field, encompassing processes across a broad range of timescales. In particular, the characteristic times associated with various combustion kinetics, (deflagration, deflagration-to-detonation transition (DDT), and detonation), injection processes (backflow and recovery), flow dynamics (residence time and mixing), wave arrival time, and acoustic modes (longitudinal and transverse resonance). This study specifically aims to explore variations in chemical kinetics time scales, given their significant impact on detonative heat release. The investigation focuses on C2H4, a higher hydrocarbon-based fuel, across equivalence ratios ranging from 0.25 to 1.25, considering three plenum pressure variations: 1, 2, and 5 atm. The chemical reaction time is typically 15 times greater than the induction time, and the chemical equilibrium time in RDE demonstrates a wider range, from 0.006 to 160 ns, depending on the inflow conditions and the fuel-mixture composition. This bears implications for optimizing detonative heat release, particularly in pre-detonation deflagration in real RDEs. Overall, this study serves as the groundwork for an extended investigation into characteristic time scales, aiming to deepen our understanding of flow physics for optimizing future RDE designs.

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Lagrangian Particle Analysis of Detonations in Stratified Reactant Mixtures

Michael Ullman, Ral Bielawski, Venkat Raman
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In many practical applications of detonation-laden flows, non-premixed reactants are supplied to the device via discrete injection. This often creates spatial and temporal variations in reactant mixedness, wherein pockets of partially premixed reactants are situated amongst regions of pure fuel or oxidizer. So call “stratified reactant mixtures” have been found to impact macroscopic wave behaviors, such as detonation cell size and wave speed, but the mechanisms driving discrepancies from ideal detonation propagation remain unclear. To address this, the present work considers two- and three-dimensional simulations of detonations traversing stratified reactant mixtures in rectangular channels. Adaptive mesh refinement and detailed chemical kinetics are used to simulate the complex induction and reaction zones with O(100) cells per notional ZND induction length. A digital filtering approach is used to generate reactant mixtures with three different stratification length scales, and the subsequent effects on wave speed, structure, and stability are analyzed. To examine how the detonation processes the nonuniform reactants, an in-situ Lagrangian particle tracking algorithm is implemented in the solver. This allows the state of notional fluid particles to be stored at runtime, such that the thermodynamic cycles experienced by fluids with different initial reactant compositions can be analyzed. These investigations thus provide translatable insights into the underlying physical phenomena dictating unsteady detonation propagation in applications of interest, such as rotating detonation engines (RDEs).

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Two-dimensional Numerical Simulation on Dimethyl Ether / Oxygen Premixture Detonation in a Narrow Channel Using Reduced Chemical Reaction Model: Effects of Numerical Accuracy on Formation of Cellular Sub-Structure

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Two-dimensional numerical simulations on dimethyl ether (DME)/oxygen detonations are performed using a reduced reaction model to investigate the effects of numerical resolution on unstable features of the cellular sub-structure. The Zhao et al. model which includes 55 chemical species and 290 elementary reactions is used in the present study. The two-dimensional simulations with different channel widths and numerical accuracy show that the detonation propagates at the CJ (Chapman-Jouguet) velocity and strongly irregular cellular structures are observed for all cases. However, the simulated mean and maximum/minimum detonation cell sizes depend on the grid resolution and the spatial order of the numerical flux. A sub-structure, associated with the transverse detonation, is captured by the higher-order scheme. This sub-structure causes a generation of many triple points because of a short induction distance between the Mach stem and the combustion front. The fifth-order WCNS (weighted compact nonlinear scheme) schemes improve the resolution near the shock wave and combustion front compared with the second-order MUSCL.

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Massless-tracer analysis of detonation-turbulence interaction in non-diluted stoichiometric hydrogen/oxygen mixture: a DNS study

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Detonation engines have extensively been studied so far, but most of the related fundamental research ignored the effect of turbulence caused by propellant injection. Our recent work performed direct numerical simulations (DNSs) of detonation-turbulence interaction and showed that turbulence collapses cellular structure and promotes reactions. As a further investigation, particle-based analysis is useful because the detonation peaky structure could not be captured via conventional time and spatial average. Therefore, in this study, DNS with newly incorporated massless tracer analysis is performed to evaluate the peaky structure and the effects of turbulences on the detonation in a non-diluted stoichiometric hydrogen/oxygen mixture in detail. The results show that the massless-tracer analysis can reproduce peaky structures and demonstrate that the distributions of inflow velocity into the shock affect subsequent structures. Also, the stronger turbulence increases the peak pressure, promotes chemical reactions, widens the distribution of inflow velocity into the shock, and shortens the induction length, which is the actual distance from the shock to the flame. Moreover, the high peak pressure under strong turbulence is caused by the region of higher inflow velocity into the shock. These suggest that the use of present analysis is effective for understanding the detailed physics of detonation in non-ideal situations. An extension to Eulerian-Lagrangian modeling with inertial particles for two-phase detonation is being planned for our future works.

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LES simulation of Tangential-mode Combustion Instability in the Rocket Combustor with Multiple Impinging-type Injectors

Bu-Kyeng Sung, Jeong-Yeol Choi
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In the present numerical simulation, the rocket combustion with 48 impinging-type injectors is simulated by using the RPL3D in-house code. The combustor was designed as a rotating detonation rocket engine by Nagoya University. Also, the combustor is experimentally assessed and confirmed operatable as an RDRE. By reviewing the design of the combustor, it is found to have undesirable design conditions which may trigger the combustion instability of the rocket combustor. This undesirable design condition, such as a large mixture distribution adjacent to the wall, for the rocket engine acts as a necessary condition for the rotating detonation engine. The gaseous Ethylene and the oxygen is used as a propellant. The quasi-global chemistry mechanism with 9 species and 10 reaction steps is used. The ignition is achieved by applying a temperature of 1800 K in the combustor. After the ignition, the combustion instability is derived without any trigger function. The combustion instability was developed over a millisecond of simulation. After the flow had fully developed, the period of pressure peaks was compared with a C-J detonation condition. The speed of the detonation wave was found to be 2239.9 m/s and compared to the CJ condition, the velocity deficit correspond to 24 % similar to most of the rotating detonation engines. Therefore, it is concluded that this rocket combustion instability is a rotating detonation.

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Numerical Analysis on Pressure Gain Combustion of Radial-Rotating Detonation Engine

A. Koichi Hayashi[1], Takumi Ito[2], Nobuyuki Tsuboi[2], Kohei Ozawa[2], Yuta Otsuka[3], Kazuhiro Ishii[3]

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Disc-type Rotating Detonation Engine (D-RDE) is useful device for a practical RDE at the point of its compactness. So far, we have been especially studying D-RDE numerically and experimentally since more than five years. The present work will show the discussion of the results, their summery, important findings, and future direction, based on Pressure Gain (PG) through our understandings from the passed studies. Furthermore, knowing the accuracy and problems of numerical analyses and the comparison between the numerical results and experimental ones, we will discuss about D-RDE to get a better PG. One of the points we will talk is some solution from the point of views of gas-turbine engine. So far, we obtained the PG values for numerical simulations as well as experiments, which provide quite good agreement with the results by the passed several researchers' studies. One of our findings from those passed PG results is that the PG values are independent from the RDE configurations such as regular RDE and Disk-RDE.

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MS07-2 Computational Tools for Detonation-Driven Propulsion Physics (2)

Chair: Jeong-Yeol Choi
Co-Chair: Nobuyuki Tsuboi
Friday, May 10; 13:00 - 15:00; Room G

3D Evaluation of H2-Air Non-Premixed Gas Injection Ports Number on Flow Field in Disk RDE

Takumi Ito[1], Nobuyuki Tsuboi[1], Kouhei Ozawa[1], Koichi A Hayashi[2]

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Detonation is a form of combustion in which combustion waves induced by a shock wave propagate through the reaction mixture. Rotating Detonation Engine (RDE), in which detonation waves rotate in an annular combustor, is said to improve theoretical thermal efficiency by more than 20% compared to the Brayton cycle. Therefore, it is attracting attention as a next-generation engine; in 2018, a Disk Rotating Detonation Engine (DRDE) was proposed, which combines a radial turbine with a high expansion ratio per stage with an RDE. Previous studies showed characteristics propagation of approaching and departing under premixed injection with hydrogen-oxygen. However, no similar propagation was observed in the case of hydrogen-air. Therefore, this study presents a three-dimensional viscosity simulation of a DRDE (disk-type rotary detonation engine) using the Navier-Stokes equations with the UT-JAXA reaction mechanism for hydrogen-air. The purpose of this study is to visualize the propagation pattern in the DRDE combustor, to investigate the effect of the number of injection ports on the propagation pattern under non-premixed injection conditions, and to evaluate the effect on stable detonation propagation and DRDE performance. These evaluations and indices such as Pressure-Gain will be used to estimate the performance of the DRDE when a turbine is inserted.

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LES Modeling and Analysis of Flow and Combustion Dynamics in a Hydrogen-air Rotating Detonation Engine Coupled with Diverging Nozzle and Turbine Stator Blades

Pinaki Pal
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A large-eddy simulation (LES) study is conducted to numerically investigate the combustion dynamics as well as aero-thermal phenomena in a non-premixed hydrogen-air rotating detonation engine (RDE) configuration coupled with a diverging-shaped lower-end wall and downstream turbine stator blades. The wall-modeled LES framework incorporates hydrogen-air detailed chemical kinetics and adaptive mesh refinement (AMR). A comparative analysis is carried out for two operating conditions with different fuel/air mass flow rates but global equivalence ratio of unity. Numerical results indicate significant deflagrative combustion occurring in the fill region. Moreover, the leading detonation wave is found to be trailed by a characteristic azimuthal reflected-shock combustion (ARSC) wave, which consumes unburned vitiated reactants that leak through the main detonation wave. A novel combustion diagnostic technique based on chemical explosive mode analysis (CEMA) is employed to quantify the fraction of heat release occurring in the detonative mode versus deflagrative mode for the simulated conditions. Lastly, analysis of combustion behavior and phase-averaged exit flow profiles is performed in the presence and absence of turbine stator blades.

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Numerical Investigation of the Interaction between the Exhaust Flow of Reflective Shuttling Detonation Combustor and Supersonic Turbulent Flow

Moeno Miyashita[1], Akiko Matsuo[1], Eiji Shima[1], Noboru Itouyama[2], Akira Kawasaki[3], Ken Matsuoka[2], Jiro Kasahara[2]
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In this study, three-dimensional numerical analyses for Reflective Shuttling Detonation Combustor (RSDC) with external main flow were conducted to investigate the new concept of RSDC for practical use. The computational targets of RSDC are the region where the hydrogen-air premixed gas flows from three rows of injectors set at the bottom in fuel-rich conditions. The main flow area is the region where the air flows at Mach number 3, and the RSDC was connected with the main flow area. The reflective wall distance, the height, and the width of RSDC were set to 45.0 mm, 53 mm, and 5 mm. The governing equations used in this study were three-dimensional compressible Navier-Stokes equation and a chemical conservation law of 9 species. The Hybrid LES/RANS model was also used as the turbulence model. As a result, the mixture of the exhaust flow of RSDC and the main flow were observed in the main flow area, and the excess hydrogen in the exhaust flow combusted. In addition to these results, the effect of the inflow angle of exhaust flow of RSDC was further investigated by analyzing additional targets, which RSDC were connected with the main flow area at different angles.

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Numerical Consideration to Geometry of Diverging Rotating Detonation Engine

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In this study, the flow structure and propulsive performance of the diverging RDEs were investigated, and its geometry was considered. The combustor length and bottom diameter were fixed at 70 mm and 20 mm, respectively, and hydrogen-air premixed gas was used as propellant. A detonation propagated stably in the straight channel, while internal pressure and combustion efficiency decreased in the diverging RDE with angle of 5 deg (position to start diverging: 0 mm). Based on these results, we searched for the optimum geometry to maintain rapid combustion and improve propulsive performance. Here, analyses for combustor geometries with 10, 20, and 30 mm of position to start diverging were conducted. Supersonic exhaust was observed in all combustors with a diverging section. In particular, in the case of 20 and 30 mm, the flow choked at the start point of the diverging, and the pressure distribution near the bottom was similar to that of a straight channel. It is considered that high combustion efficiency can be maintained by diverging the flow path behind the detonation, where combustion proceeds rapidly. In addition, the relationship between the combustion region, geometry, and propulsive performance was summarized, and guidelines were obtained for optimal design.

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A low-dimensional modeling approach to acceleration of an internal flow of a rotating detonation engine

Kotaro Nakata[1], Noboru Itouyama[1], Ken Matsuoka[1], Jiro Kasahara[1], Akira Kawasaki[2], Hiroaki Watanabe[3], Akiko Matsuo[4], Ikkoh Funaki[5], Kazuyuki Higashino[6]
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A quasi-one-dimensional flow model for an internal flow of a rotating detonation engine (RDE) with multiple diverging angles (constant diverging angles from −3 to 5 deg) was proposed to reveal its acceleration mechanism. An RDE without an inner cylinder that had an inlet diameter of 20 mm was focused on, and gaseous ethylene-oxygen or hydrogen-oxygen was utilized as the propellants. In a diverging channel, a subsonic flow near the injector surface was accelerated via heating from a detonative combustion, choked around the middle of the channel, and then accelerated to supersonic speed. In the converging channel, a smaller exit area resulted in a higher pressure, and a subsonic flow was gradually accelerated to be sonic speed at the exit due to mechanical converging. To validate the model, experimental results from pressure measurements and optical observations were introduced. Axial pressure distributions in the calculation and in the experiments had the same tendency, and high-speed images captured from the side of the RDE implied a compact heat release region near the injector surface as estimated in the calculation. These results suggested that the internal flow of the RDE can be reasonably estimated by the quasi-1-D model.

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MS08 Advances in Detailed Numerical Simulation of Reciprocating Engines

Organizers: Yasuo Moriyoshi[1], Taisuke Nambu[2]

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MS08 Advances in Detailed Numerical Simulation of Reciprocating Engines

Chair: Yasuo Moriyoshi
Co-Chair: Taisuke Nambu
Wednesday, May 8; 10:40 - 12:20; Room J

Research and Development of a Combustion Flow Analysis Program for Reciprocating Engines Using the Cartesian Grid and an Immersed Boundary Method

Taisuke Nambu[1], Hiroki Yao[2], Takuhito Kuwabara[3], Ryohei Kirihara[3], Yasuhiro Mizobuchi[1]

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This presentation shows ongoing research and development efforts on the combustion flow analysis program, HINOCA, with a focus on detailed simulations of reciprocating engines using large-scale computer. A bottleneck in performing detailed combustion flow analysis of motoring and firing of reciprocating engines is the computational grid generation cost associated with geometry motion. The analysis program uses the Cartesian grid method and an Immersed Boundary (IB) method, which significantly reduces the computational grid generation cost and achieves good performance in large-scale parallel computation. However, the use of the Cartesian grid and IB method is known to cause problems such as reduced accuracy near shape walls and poor conservatism. Ongoing research and development efforts are underway to improve these aspects.

This presentation provides an overview of the analysis methodology used by HINOCA, including analysis examples. The analysis based on the Cartesian grid method and the IB method shows that it is possible to analyze reciprocating engines with many complex geometries with the same or better accuracy than the analysis using a conventional boundary-fit grid method.

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Conceptual Study of High Efficiency Reciprocating Engine with Pre-chamber Combustion

Takayuki Ito[1], Masahiro Matsuoka[1], Toru Takabayashi[2]

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This presentation shows ongoing conceptual study of the spark ignition engine by using combustion flow analysis program HINOCA, which uses the Cartesian grid method and an Immersed Boundary (IB) method and involves many physical and chemical sub models to represent the complex phenomena in engine combustion. HINOCA provides the useful information to explore the newly method for improving the engine combustion such as the suppression of the cycle-by-cycle variation with its scalability on the large-scale computer. We focus on the use of active type of pre-chamber which enables to enhance the lean limit for highly efficient lean combustion. The pre-chamber combustion has potentiality for significant reduction of the combustion instability when the ultra-lean premixture is applied to aim the achievement for high-efficiency gasoline engines. Furthermore, we found that the utilization of the autoignition around the jet flame improves the thermal efficiency due to rapid combustion and reduction of the unburnt fuel near the in-cylinder wall.

This presentation introduces the recent our parametric study for the effects of the compression ratio and in-cylinder condition such as gas composition on the heat release rate profile and the potentiality for the improving the thermal efficiency.

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Approach to Carbon Neutral Fuel Engine Combustion Analysis Using Ansys Forte and Model Fuel Library

Junya Fukuyama

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As countries around the world move toward carbon neutrality, the transportation sector, including passenger

cars (two-wheeled and four-wheeled), trucks, and ships, construction machineries, and agricultural machineries, as well as stationary generators are required to switch to alternative fuels that reduce CO_2 emissions. Under such circumstances, hydrogen engines are attracting attention as a new alternative to conventional diesel and gasoline engines. In this presentation, the three-dimensional combustion simulation approach will be explained, which is one of the essential simulation technologies for hydrogen engine development. Ansys has been working on combustion simulation for carbon-neutral fuels for many years. Fuel modeling is also important to appropriately express the combustion process, Ansys has built a Model Fuel Library and uses these fuel characteristics to perform combustion analysis with Ansys Forte. The latest development efforts and simulation examples for hydrogen engine combustion in Ansys will be demonstrated.

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Numerical Analysis of Soot Contamination Process in Diesel Engine Combustion

Tsukasa Hori[1], Shohei Ueno[2], Shinya Sawada[2], Fumiteru Akamatsu[1]

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Combustion improvements and the use of after-treatment systems have reduced soot emissions from engines. On the other hand, depending on the engine conditions, soot may be introduced into the engine oil due to impingement of the spray flame on the combustion chamber liner, resulting in deterioration of the engine oil performance. In the case of diesel engines, it is believed that soot adheres to the engine oil film on the cylinder liner wall due to the impingement of the spray flame on the wall, and that the sliding motion of the engine piston transports the soot to the oil pan, where it is mixed into the engine oil. However, although prediction models have been developed for soot itself, few models have been developed for soot deposition on walls. The objective of this study was to predict soot contamination of oil in diesel engines. An engine combustion simulation code developed by the authors was used for the calculations. PRFs of cetane and isocetane were used as the fuel reaction mechanism. PAH formation by gas phase reaction is considered up to pyrene. Soot formation from pyrene was calculated using the method of moments. Then, a soot adhesion model that takes thermophoretic motion into account was developed for the moment method and incorporated into the numerical analysis code. Numerical calculations were performed for engine conditions in which soot contamination with engine oil was measured, and the accuracy of the calculations was examined.

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MS09 Numerical Combustion Research on Fundamental Phenomena in Automobile Engines

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MS09 Numerical Combustion Research on Fundamental Phenomena in Automobile Engines

Chair: Shinji Nakaya
Co-Chair: Tsukasa Hori
Thursday, May 9; 09:50 - 12:10; Room J

Numerical analysis of the initial flame kernel development with spark channel elongation in spark ignition process under turbulent tumble flow conditions using LES/FGM

Shinji Nakaya, Fangsi Ren, Mitsuhiro Tsue
The University of Tokyo, Japan

A numerical simulation model on the spark ignition process in lean-combustion spark ignition (SI) engines operating under high flow speed turbulent conditions was developed. The model employs Large Eddy Simulation (LES) coupled with a tabulated chemistry based on the flamelet generated manifold (FGM). The numerical model incorporates the elongation, restrike, and shortcut models of the spark discharge channel, considering the electric circuit and the spatial distribution of local electric fields. Three-dimensional LES simulations were conducted to investigate the spark ignition process in turbulent tumble flows for lean gasoline or ethanol mixtures in a rapid compression machine, operating at elevated temperatures and pressures. The results indicated that the numerical model successfully reproduced elongation, shortcut, and restrike behaviors observed in experimental studies. Qualitative agreement with experimental data was achieved in the initial flame kernel development, even with a tabulated chemistry of Flamelet-Generated Manifold (FGM) models. The size of the flame kernel was confirmed well with the experimental one. Additionally, the numerical results represented local quenching behaviors observed in the experiments, demonstrating the model's capability to capture detailed combustion phenomena. The influence of Lewis number on the spark ignition process was also explored in the present study.

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Effect of flame quenching distance and flame-wall geometry on the near-wall CO formation for turbulent premixed CH4-air combustion in a constant volume vessel

Ye Wang, Mamoru Tanahashi
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A three-dimensional direct numerical simulation has been conducted for the turbulent premixed CH4-air combustion in a constant volume vessel. The local near-wall flame quenching positions of turbulent flame-wall interaction process are identified based on the flame's local fuel consumption speed, and the CO emission of near-wall flame is investigated for its correlation to the local near-wall flame quenching distance and flame-wall geometry. The results show that, the local flame gets near-wall quenched primarily with a head-on quenching configuration. Meanwhile, the physical barrier effect of wall causes the "lack of fuel" in the flame front and that further leads to the statical reduction of CO emission during the near-wall flame quenching process. Additionally, the CO emission exhibits dependence on both local quenching distance and quenching mode (flame-wall geometry): a greater level of CO emission rate can be found on the near-wall flame with a longer quenching distance or under quenching mode of back-on quenching (flame oriented far from the wall), as the flame front can be better exposed to the unburned mixture. Moreover, the behaviors of CO-related elementary reactions are also investigated to support the current findings.

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Combustion characteristics of ammonia-hydrogen mixtures by turbulent jet ignition

Dong Han, Jinlu Huo
Shanghai Jiao Tong University, China

Ammonia, as a hydrogen carrier and zero-carbon fuel, holds promise for achieving zero carbon emissions from internal combustion engines. The pre-chamber turbulent jet ignition, characterized by multi-point distributed ignition and rapid combustion, could be applied to ammonia combustion to extend combustion limits and stability. This study investigates the impacts of hydrogen energy fraction and equivalence ratio on the ammonia-hydrogen mixtures jet ignition in a constant volume combustion chamber with pre-chamber ignition system by CFD Simulation. The results indicate that, with high hydrogen content and near-stoichiometric combustion conditions, the flame thickness decreases. This allows the fire nucleus to penetrate the main-chamber, even with the jet hole stretching effect and heat loss, forming the flame ignition. When the hydrogen energy fraction decreases or the equivalence ratio drops, the increased flame thickness lead to the pre-chamber flame being easily and completely quenched as it passes through the jet orifice, resulting in the formation of a jet into the main-chamber that contains only the combustion thermal products. In comparison to the flame ignition, the jet ignition demonstrates a prolonged ignition delay time, with ignition occurring at the jet tip, distanced from the pre-chamber outlet. Therefore, the hot jets formed by ammonia-hydrogen fuel mixtures with high hydrogen ratios or stoichiometric mixtures provide advanced main-chamber mixture ignition and stronger jet flow.

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Numerical Simulation of Spark Ignition Processes Considering Preferential Diffusion and Thermal Plasma

Tsukasa Hori[1], Naohiro Yoshinaga[1], Shota Yamada[2], Yusuke Oda[1], Shinya Sawada[1], Fumiteru Akamatsu[1]
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In order to improve the thermal efficiency of spark-ignition engines, there is a need to predict the success or failure of spark-ignition and flame kernel growth for lean mixtures. In recent years, the prediction of sub-chamber ignition and ignition for mixtures of hydrocarbon fuel, ammonia and hydrogen have become promising. It is required to predict the preferential diffusion effect appropriately for the mixing composition in addition to improving the prediction of spark discharge such as discharge path elongation and re-discharge. Preferential diffusion effects can be taken into account by considering multi-component transport properties. On the other hand, the simulation considering plasma requires time resolution to capture the transfer of electrons. From the viewpoint of computational load, it is difficult to predict from the start of discharge to the flame kernel growth. In this study, we developed an numerical simulation method of spark ignition process that takes thermal plasma into account. By assuming local equilibrium and considering spark ignition plasmas as thermal plasmas, flame kernel growth calculations can be performed without changing the calculation time scale due to the introduction of plasma. In addition, the simulation considering thermal plasma predicts the elongation process of the discharge path and the flow associated with the discharge. In this talk, we will introduce the development of a numerical simulation for spark ignition that takes into account preferential diffusion effects and thermal plasma, and the simulation results of spark discharges and flame kernel growth.

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Autoignition behaviour of n-heptane studied using 2D DNS

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This work presents 2D DNS study at higher initial temperatures where the end-gas autoignition changes its nature. The autoignition center moves away from the end wall as the initial mixture temperature increases. This is attributed to the multiple reflections from the side walls in 2D enclosure due to which higher temperature region is created inside the domain and away from the wall. As the initial temperature increases from 1100 K to 1200 K autoignition kernel moves further away from the end-wall. In 2D DNS, the autoignition is initiated at significantly lower level of temperature inhomogeneity as compared to 1D DNS. The autoignition modes are also influenced by increase in pressure. The autoignition center moves towards spark ignited flame front as the pressure increases and new modes are observed at significantly higher pressure.

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Prediction of Knock Intensity for an Optical SI Engine with Various Primary Reference Fuels

Jiabo Zhang[1], Shi Hao[2], Dong Han[1], Zhen Huang[1]
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To provide fundamental insights into the underlying mechanisms of knock occurrence in a spark-ignition (SI) engine, optical diagnostic measurements were performed at advanced spark timing under boosted conditions. Employing high-speed imaging, deflagration-to detonation transition (DDT) processes were recorded. The relationships between the unburned mixture fraction (UMF) and two metrics associated with the knock intensity levels, namely the maximum amplitude of pressure oscillation (MAPO) and the peak in-cylinder pressure, Pmax, were examined. In contrast to common beliefs, we found that the knock intensity represented by MAPO is not strongly correlated with UMF, because UMF alone is inherently insufficient to represent the thermo-chemical properties of the bulk mixture inhomogeneities and its chemical reactivity at the onset of end-gas autoignition occurrence. Instead, a much stronger correlation was found between UMF and a newly proposed normalized-peak-pressure metric, allowing an a prior prediction of Pmax, which is a critical parameter associated with the propensity of engine failure if Pmax exceeds the strength limit of the engine. To quantitatively predict MAPO under SI-engine conditions, a refined model was proposed by imposing the pressure and temperature traces into the zero-dimensional (0-D) reactor model, such that the thermochemical properties of the transient mixture state at the onset of end-gas autoignition are properly incorporated into the predictive criteria. The model is proved to reliably predict the end-gas autoignition and the knock intensity levels dictated by MAPO regardless of the stochastic nature of the knock development process and fuel types.

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Numerical investigation of the effect of combustion process on material thermal load under internal combustion engines conditions

Chunkan Yu, Ulrich Maas
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While thermo-mechanical analysis in solids and combustion processes in the gas phase have been intensively studied separately, their interaction is less investigated. This talk focuses on the coupling between processes in the solid phase and the gas phase during a combustion process. The influence of the solid on the flame structures and flame properties as well as the influence of the flame on the thermo-mechanical behavior in the solid are investigated with the focus on internal combustion engines conditions. A stagnation flow flame close to a plane wall is considered as a representative model, which is simple but also relevant for many engineering conditions. The numerical simulation of the combustion process is based on detailed chemical mechanisms and detailed molecular transport models including thermal diffusion. The model for the solid is based on the thermo-elasticity assumption. We present a fully coupled solution of the governing equations for the solid and the gas phase. As a result, it is shown that the plane wall (e.g. its heat conductivity) can significantly affect the flame properties (e.g. its stability against extinction), and the flame, in return, can affect the thermal stresses in the plane wall, and the solid is more likely to undergo a plastic deformation at high pressures.

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MS10 Sustainable Aviation Fuel: Modeling Challenges and Opportunities

Organizers: Shashank Yellapantula[1], Jacqueline H Chen[2]

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MS10 Sustainable Aviation Fuel: Modeling Challenges and Opportunities

Chair: Shashank Yellapantula
Co-Chair: Jacqueline H Chen
Friday, May 10; 09:50 - 11:50; Room C

Challenges and Opportunities in Using Numerical Simulations for Increased Adoption of Sustainable Aviation Fuels

Shashank Yellapantula, Bruce Perry, Sreejith Nadakkal Appukuttan, Marc Day
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Liquid fuels from bio-derived sources, sustainable aviation fuels (SAF), are currently the most promising avenue to decarbonize aviation. Currently, there are seven fuels produced from various sustainable feedstocks that are certified to use in commercial aviation in US. All of these seven fuels, also known as drop-in fuels, need to be blended with petroleum based jet fuels at various blend ratios, maximum being 50%. In order to achieve significant decarbonization several 100% drop-in fuels need to be certified and the production process scaled up to millions of gallons. However, cost and amount of fuel needed for certifying a new synthetic fuel presents a major challenge. To de-risk certification of 100% drop-in SAF, simulations provide a cost-effective alternative to screen several fuel candidates in a time efficient and cost-effective manner.

In this mini-symposium, we will highlight challenges and opportunities for simulation of aircraft engine combustors with a specific goal of faster and cheaper routes to adoption of 100% SAF. As a part of this mini-symposium, this first talk will introduce the concept of drop-in SAF, the SAF certification process, and highlight the risks associated with this process. Additionally, the talk will highlight the critical role that simulations can play to de-risk and reduce costs of newer SAF certification. Finally, the talk will introduce all the following talks where all aspects of modeling challenges associated with SAFs will be discussed.

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Modeling sustainable aviation fuel combustion kinetics with a functional group approach

Pierantonio Lo Greco[1], Sirio Brunialti[1], Qi Wang[1], Xiaoyuan Zhang[2], **Mani Sarathy**[1]
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Sustainable aviation fuels have the potential to replace conventional petroleum derived fuels in long-haul flights. The chemical composition of SAFs determines their combustion properties and performance in flight. It is important to determine how feedstock variability and variations in SAF production processes impact fuel chemical composition and combustion kinetics. Here, we present a functional group approach to (FGMech) simplify the kinetic modeling of SAF combustion. The FGMech methodology enable rapid development of reaction mechanisms, thermodynamic data, and transport data for real fuels with complex chemical composition. The FG-Mech approach is used here to develop kinetic models for conventional Jet-A1 and SAFs produced by hydrotreating of fatty acids (HEFA). The kinetics models are validated by comparing predicted results of C2H2 and C3H4 with experimental shock tube measurements. Subsequently, the kinetic model is merged with a PAH formation mechanism and results are compared with simple reactor experiments. Finally the mechanisms for NOx, sulfate and nucleation-growth-oxidation of soot are added. Furthermore, the FGMech models are applied to simulate emissions from a turbofan (with emphasis on NOx, CO and soot). The emission model also implements a variable distribution of mass flow rates in the burner as a function of engine operating conditions. The model's predicted values are compared with experimental measurements from NASA APEX and ACCESS campaigns to assess the model's accuracy.

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A perspective on supercritical fuel-flow modeling needs with SAF

Guillaume Ribert
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The critical point of any pure substance can be defined by the highest pressure and temperature, for which distinct liquid and gas phases can be observed. When the pressure exceeds such critical pressure, the distinction between gas and liquid vanishes, and real-gas effects must be addressed. For binary and other multicomponent fluids, several locations of critical points are found depending on the concentration of each fluid. Such phenomena are classically encountered in rocket engine applications but can also appear in gas turbines, particularly if sustainable aircraft fuels (SAF) are used. This high level of pressure has a direct impact on the flow Reynolds number through the kinematic viscosity. The Reynolds number increases with pressure involving a decrease of the Kolmogorov scale with consequences on the mesh requirements. Furthermore, under these severe thermodynamical conditions, flames become very thin with steep density gradients, meaning a modeling effort is required for both turbulent flow description and propulsion applications. An overview of the different challenges related to this research theme will be detailed in the context of using SAF for aeronautical propulsion.

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Toward comprehensive manifold-based combustion modeling of multi-component Sustainable Aviation Fuels in turbulent reacting flows

Michael Edward Mueller, Israel J Bonilla, S Trevor Fush, Philip Satterthwaite
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Multi-component liquid fuel combustion poses several computational modeling challenges. Multiple fuel components requires the use of large chemical mechanisms, which are generally computationally intractable with "brute force" combustion modeling approaches so requires reduced-order manifold-based combustion models. The fuel components may have varying rates of vaporization, so the manifold-based model must accommodate a diversity of local fuel compositions, increasing model dimensionality. Additionally, liquid fuel combustion with varying vaporization rates can exhibit complex multi-regime combustion. In this work, progress toward a comprehensive manifold-based combustion model for multi-component liquid fuel combustion is detailed. To accommodate varia-

tions in the local fuel composition, the local fuel composition is considered as an input to the manifold-based model. The importance of the local fuel composition on the thermochemical state is demonstrated with a particular emphasis on emissions. To accommodate this relatively high-dimensionality of the manifold-based model, In-Situ Adaptive Manifolds (ISAM) computes solutions to the manifold equations 'on-the-fly' and stores them for reuse later in the simulation. The performance and scalability of ISAM in LES with chemical mechanisms of varying size from ten species to hundreds of chemical species and with different "fuel" dimensionalities are assessed. Finally, generalization of the model to complex multi-regime combustion is discussed including both multi-modal combustion and quasi-staged combustion.

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Experimental Approaches for Validation of SAF Combustion

Tonghun Lee, Audrey Godsell, Casey O'Brien, Paxton Wiersema
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This presentation will outline an effort to develop a new compact test rig (M1 combustor) for prescreening sustainable aviation fuels (SAFs) prior to tier 3 and 4 tests in the ASTM D4054 evaluation process. The M1 combustor is designed to operate on a small quantity of fuel, and its combustion characteristics for various fuels are characterized using state-of-the-art laser and optical diagnostics including multiphase X-ray measurements at the Advanced Photon Source (Argonne National Laboratory). The goal is to provide an open architecture that can be utilized for prescreening of SAF as well as provide high-fidelity data for validation of numerical models. Combustor test results of lean blow out and ignition, based on a variety of fuels with varying properties representative of SAF, will be presented. Additionally, the presentation will cover some of the latest work in rapid optimization of chemical kinetics models for SAF which can be utilized in modeling the M1 combustor. This includes utilizing advanced machine learning based analysis to understand the uncertainty space when models are optimized using limited experimental data.

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Combustion dynamics in a lab-scale combustor using DNS

Bruno S. Soriano, Christian Lacey, Jacqueline Chen
Sandia National Laboratories, United States

The combustion process in aero-engines is a result of complex interactions between multi-phase flows with different fuel properties, mixture preparation in turbulent flows and complex chemical reactions. The liquid injection of multi-component fuels often results in partially-premixed mixture preparation which can also vary in terms of fuel composition and generate complex multi-mode combustion. Fuel pyrolysis and mixing of the various fuel fragments with the local mixture increases the dimensionality of the problem. The presence of extinction and reignition in stringent conditions near flame blow-off increases the difficulties to correctly model the combustion process for engineering simulations. The flame sensitivity to blow-off has been observed to be related to the fuel propensity to ignite, measured in terms of the derived cetane number. In this work, combustion dynamics involved in jet fuel combustion is investigated using a laboratory-scale swirl-stabilized spray flame modeled using direct numerical simulation. Simulations are performed for two fuels with dissimilar cetane numbers: the first with the commercially available Jet-A; and the second with Alcohol-To-Jet, a low cetane number Sustainable Aviation Fuel (SAF) called C1. The combustion dynamics is investigated in terms of the combustion modes and the propagation mode of the edge flames generated from local extinction at the stoichiometric mixture fraction. Statistics in terms of the edge flame displacement speed are also analyzed for the two fuels. Finally, modeling closures in the context of multi-modal combustion are discussed.

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MS11 Liquid Rocket Engine Combustion

Organizers: Takanori Haga[1], Taro Shimizu[1], Hiroshi Terashima[2]

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MS11 Liquid Rocket Engine Combustion

Chair: Taro Shimizu
Co-Chair: Hiroshi Terashima
Thursday, May 9; 09:50 - 12:30; Room G

Large-Eddy Simulations of subscale LOX/GH2 rocket combustors with different fuel injection temperatures

Takanori Haga, Taro Shimizu
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Large-eddy simulations are performed for subscale rocket combustors by solving the compressible Navier-Stokes equations with the flamelet progress variable model. To account for real-gas thermodynamics and transport of the cryogenic propellants, the Soave-Redlich-Kwong equation of state and Chung's model are used. In-house solver "LS-FLOW-HO" is used, in which the high-order flux-reconstruction scheme is employed on overset unstructured hexahedral grids.

First, a single coaxial injector case tested at JAXA Kakuda Space Center is considered. To reproduce the injector acoustic modes with proper upstream boundary conditions, the geometry of the injection manifolds is included in the simulation. The computed power spectral density (PSD) of the pressure was compared with the experimental data, and the overall characteristics agreed reasonably well. In the higher amplitude case, interference between LOX core and GH2 annular flow occurred in the recessed region at the injector end, and coupling of the core deformation and the injector 1L mode was observed.

Next, LES of DLR BKD 42 injectors is conducted. In the experiment, higher amplitude of 1T mode was observed in the higher hydrogen temperature case LP4. The computed combustion pressure and the PSD will be compared with the experiment and the characteristics of the combustion flow field will be discussed.

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Injection parameter identification for severe pressure oscillations in a high-pressure H2/O2 rocket-type chamber

Riku Shimoyama, Atsushi Kubota, Hiroshi Terashima
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Combustion instabilities are a severe problem for developing liquid rocket engines. The combustion instabilities may generate large pressure oscillations, causing severe damage to the combustion chamber. This study numerically investigates the effects of injection velocity and mixture ratios on the combustion instability in H2/O2 rocket-type engines with low-temperature injection. The compressible Navier-Stokes equations, including the species-mass equations, are solved with a detailed chemical kinetic mechanism. The results indicate that the combustion instabilities with strong pressure waves are generated under low-velocity or low mixture ratio conditions. The instability conditions using the velocity and mixture ratios agree with several experimental data. The results also suggest that the low-temperature injection may not be a primary cause of the combustion instabilities. When strong instabilities occur, some unburned hydrogen remains downstream. The local Rayleigh index indicates that the unburned hydrogen remaining in a downstream region causes the interaction between the exothermic fluctuations by combustion reactions and pressure fluctuations in a chamber. Therefore, the present study suggests that the unburned hydrogen remaining downstream is a primary cause of the combustion instabilities with strong pressure waves. The injection velocity and mixture ratios, which indicate the amount of unburned hydrogen downstream, are a metric for predicting combustion instability.

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Characterization of injectors near field in LRE firing plates

Pasquale Eduardo Lapenna[1], Arianna Remiddi[2], Marco Pizzarelli[3], Rocco Pellegrini[3], Enrico Cavallini[3], Mauro Valorani[2], Francesco Creta[2]

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Liquid Rocket Engines (LRE) are usually characterized by extreme conditions in terms of temperature and pressure, making the experimental investigation of such devices complex and often limited to indirect measurements. The injection region, in particular, lacks a thorough description from both the experimental and numerical standpoints. In this framework, the interest toward variable-fidelity computational fluid dynamics (CFD) simulations is rapidly increasing with a twofold aim. On one hand, high-fidelity simulations such as large eddy simulations (LES) and direct numerical simulation (DNS) can provide data and information which are typically hindered to experiments. Low-fidelity simulations like unsteady RANS, on the other hand, can be used to characterize large and complex domains and to develope reduced order models for simulations at the system level. This contribution aims at the characterization of the injectors near-field region of rocket combustion chambers, with particular attention devoted to the mixing and recirculation region, and comprising the effects of the injector layout on the ensuing flow field and thermal load. The work will leverage the use of a tabulated chemistry approach coupled with multi-fidelity solvers ranging from unsteady RANS to LES, and will be based on reference test cases widely validated in the rocket community.

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Modeling of Wall Heat Flux in Liquid Rocket Engines

Matthew Harvazinski

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Heat transfer plays an important role in liquid rocket engines, a large amount of heat is transferred from the combustor to the walls of the engine. Walls can also play an important role in the thermal management of the device because of regenerative cooling. Accurately modeling the wall heat transfer is difficult because of the added resolution and sophistication of the models required. In this study we look at using both conjugate heat transfer and radiation heat transfer to capture the wall heat flux in a laboratory scale rocket engine. Simulations show that to accurately capture the wall heat flux you must capture the thermal boundary layer, account for the chemical reactions taking place in the near wall region, model the heat transfer into the solid wall, and account the radiation loss inside the combustor. For example, simulations without reactions can lead to errors of 2-5 times in the wall heat flux. In this study a series of simulations is done using different levels of fidelity to demonstrate the resolution and models required to accurately capture the wall heat flux in a liquid rocket engine.

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Determination of the Drop Size and Distributions during Liquid Injection: Impinging and Effervescent Sprays

Jungeun Park, **T.-W. Lee**

Arizona State University, United States

Determination of drop size is important in propellant and other injection processes. Evaporation and subsequent combustion are predicated on the initial drop diameter and its distributions. For this reason, many models exist. In place of modeling, we have developed an analytical framework based on integral form of the conservation equations, which leads to an expression for the Sauter mean diameter as a function of the injection and fluid parameters. This has been validated for the basic injection geometries, and in this work we demonstrate extension and applicability to spray flows for propellant injection: impinging and effervescent sprays. Again, the results are compared with experimental data. In addition to providing quantitative predictions of the drop size and distributions, physical mechanisms of the spray atomization processes can be understood withing this framework. For impinging sprays, it is the cancellation of the lateral momentum and kinetic energy that leads to the formation of small droplets. This algorithm can also be combined with computational fluid dynamics for efficient and accurate simulations of propellant injection.

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An efficient numerical algorithm for solving multi-component real fluid flows in rocket engines

Sho Wada[1], Reo Kai[2], Abhishek Lakshman Pillai[1], Ryoichi Kurose[1]

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To reduce the development costs and improve the reliability of rocket engines, model-based development is necessary, which uses numerical simulations in the early design stage to evaluate the stability and efficiency

of rocket engines under operating conditions. However, numerical simulations of transcritical fluids in rocket engines suffer from the small time-step size limitation due to the acoustic CFL number and numerical instabilities arising from spurious pressure oscillation at the material interface, which lead to high computational costs and divergence of calculations, respectively. To address these issues, using a semi-implicit algorithm employing a method to mitigate spurious pressure oscillations at material interfaces appears to be a promising approach. In this study, a semi-implicit pressure-based solver that reduces the computational cost by over 90% compared with the classical explicit density-based solver has been developed for multicomponent real-fluid inert systems. This is a preliminary step towards our goal of applying this algorithm to the transcritical combustion field in the future. The validity of the developed algorithm is tested with benchmark 1D and 2D numerical problems, and its results and computational cost are compared with those of the classical density-based explicit solver.

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Interface-Capturing Simulations of Transcritical LOX/GH2 Injection using Unified-Fluids Regularized-Interface Method

Nguyen Ly, Matthias Ihme
Stanford University, United States

In modern rocket engines, cryogenic propellants are injected into a high-pressure combustion chamber to maximize thermodynamic efficiency and performance. Specifically, examples of LOX/GH2 injection engines operating at supercritical pressures with respect to the critical point of oxygen are found in the main-stage engines of SLS and Ariane 6. Despite the wide adoption, the physical mechanisms for mixing between LOX and GH2 streams remain poorly understood. One principal issue is the immiscibility of oxygen and hydrogen, resulting in the existence of liquid/vapor interfaces even at arbitrarily high-pressure conditions, when the surface temperature is below the mixture critical point. Thus, the investigation of the spatio-temporal transition of the LOX/GH2 surface between subcritical evaporation and supercritical mixing remains an open challenge. To address this, we present a Regularized-Interface Method (RIM) that was derived from up-scaling the nanoscale interface-resolving methods based on the Linear Gradient Theory of Van der Waals, thus allowing for the unified interface-capturing simulations of both subcritical interfacial and supercritical mixing dynamics. Using this method, we numerically analyze the complex spatio-temporal transcritical transition dynamics exhibited by the LOX/GH2 surface due to the inhomogeneities generated by injection.

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MS12 Spread of ammonia combustion research - Role of numerical simulation -

Organizers: Hisashi Nakamura[1], Ekenechukwu C Okafor[2]

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MS12-1 Spread of ammonia combustion research - Role of numerical simulation - (1)

Chair: Hisashi Nakamura
Co-Chair: Ekenechukwu Chijioke Okafor
Wednesday, May 8; 10:40 - 12:40; Room D

Secondary Air Dilution of the Primary Combustion Zone of Two-Stage Rich-Lean Ammonia Combustors; A Numerical Study of the Effects on Emissions Control

Ekenechukwu Chijioke Okafor[1], Hirofumi Yamashita[2], Osamu Kurata[3], Norihiko Iki[3], Takahiro Inoue[3], Hyun Jo[3], Masayasu Shimura[3], Taku Tsujimura[3], Akihiro Hayakawa[2], Hideaki Kobayashi[3],

[1]Kyushu University, Japan, [2]Tohoku University, Japan, [3]National Institute of Advanced Industrial Science and Technology, Japan

Experimental studies in two-stage gas turbine combustors suggest that the secondary air injected downstream of the combustor may flow towards the primary zone for sufficiently large secondary air flow rates. This diluting effect of the secondary air on the primary zone may limit the potentials of two-stage rich-lean combustion and inhibit flame stabilization. In this study, large eddy simulations of flows in models of two-stage gas turbine combustors were conducted using a reduced reaction mechanism to study the effects of the uncontrolled primary zone dilution on ammonia-methane-air combustion and emissions control at various primary zone equivalence ratios. It was found that the dilution event encouraged NOx emission due to non-uniformity of the mixture in the primary zone. By controlling the flow of secondary air towards the primary zone, a higher combustion temperature and a more uniform equivalence ratio in the primary zone were achieved, which enabled a better control of NOx emission. However, emissions of unburned fuel species such as NH3, H2, HCN and CO could be encouraged when primary zone dilution is mitigated because of insufficient mixing of the hot gases from the primary zone and the secondary air in the secondary zone. It was found that the emission of N2O from two-stage rich lean combustors is mainly due to its production in the secondary zone.

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Effect of Secondary Fuel Injection in Ammonia / Natural Gas Co-Fired Gas Turbine Combustor

Shintaro Ito, **Masahiro Uchida**, Yusuke Komatsu, Toshiro Fujimori

IHI corporation, Japan

Ammonia is gaining recognition as a fuel for CO2 reduction, but technology development is required to establish and expand the value chain. Especially, development of low NOx combustion technology is crucial to promote the use of ammonia as a fuel. In this study, technology to co-fire 20% ammonia with natural gas for 2 MW-class gas turbines was developed. Two-stage combustion method is adopted for ammonia / natural gas co-firing to achieve low NOx combustion. Through computational and experimental study using two-stage combustor, the effect of ammonia supplying point on NOx emission was investigated. In the computation, detailed reaction mechanism was used to investigate the process of low NOx combustion. Comparison of numerical results showed that NOx emissions were lower when all ammonia is supplied to the secondary zone than when it is supplied to the primary zone. Comparison of flame structure suggested that oxygen concentration in the ammonia combustion zone affects NOx emission. Engine tests results using a 2 MW-class gas turbine confirmed a same tendency as a numerical simulation. These results clearly demonstrated the effectiveness of secondary ammonia injection in reducing NOx emission.

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Multi-Scalar Flamelet Approach for Simulating Ammonia Co-firing Burners

Kozo Aoki, Hiroyuki Takeishi, Keisuke Miura, Kenji Yamamoto
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The objective of this work is to construct and verify the two-stream premixed flamelet approach in gas-gas dual fired burners. A numerical framework using large eddy simulations (LES) combined with Flamelet Generated Manifolds (FGM) are applied to ammonia-methane flames. Premixed flamelet library for ammonia-methane combustion is constructed with two mixture fractions (ZNH3 and ZCH4) since partially premixed combustion mode with locally different ammonia-methane ratio appears in actual gas turbine combustors. A model swirl burner in the literature, which has fuel supplying lines for ammonia-air and methane-air mixtures individually, is selected for verification of the LES. A progress variable (C) and additional non-dimensional parameters, Z=ZNH3+ZCH4 and A= ZNH3/Z, are defined to construct a flamelet library in (Z, C, A) space. Turbulence-chemistry interaction in the subgrid scale is considered by using presumed beta PDF for the variances of Z and C. Thus, the tabulated quantities are parametrized by five parameters (Z, C, A, Z", C"). LES of the elemental burner under the literature condition (21% overall NH3 ratio) successfully reproduces the flame shape represented by OH-PLIF images. Differences in the results between the present flamelet approach and detailed chemistry are also discussed in statistically.

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Numerical Investigation of Secondary Injection System in Developing Low-NO Ammonia Co-combustion Furnaces with Detailed Chemistry and Conjugate Heat Transfer

Yinan Yang, Tsukasa Hori, Shinya Sawada, Fumiteru Akamatsu
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In the context of utilizing ammonia for co-firing power generation, the air-staged strategy is recognized as an effective method for controlling NO emission due to its ability to stage air input, thereby creating a fuel-rich region within the furnace. To investigate the NO formation and reduction characteristics under various conditions within an air-staged strategy employing the secondary injection system, the present study utilized three-dimensional numerical simulations to investigate the impact of the secondary nozzle diameter (D2) and the secondary air ratio (λ2). The conjugate heat transfer (CHT) method is utilized to accurately simulate thermal conditions at the furnace walls. Results indicate that with a constant total air ratio (λ = 1.2), simply increasing the secondary air ratio, which promotes fuel-rich combustion in the primary combustion zone, does not correspond to a linear decrease in NO emission at the furnace outlet. Instead, as the secondary air ratio increases, NO emissions at the furnace outlet follow a V-shaped trend, minimizing when primary and secondary air ratios are equivalent. Additionally, increasing the secondary nozzle diameter, thereby enhancing fluid recirculatory motion, proves to be an effective means of suppressing NO emissions. This study underscores that adjustments in the secondary injection system parameters can significantly control NO formation, even without extensive structural modifications to existing combustion furnace infrastructure.

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Numerical simulation of high-temperature air / ammonia / methane mixing combustion for industrial furnaces

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Ammonia is one of the promising fuels for future zero-carbon industries. By introducing ammonia as a fuel for industrial furnaces, huge amounts of carbon dioxide emissions from industrial furnaces can be reduced in the future. In this study, the numerical simulations were conducted for the high-temperature air / ammonia / methane mixing combustion field of the lab-scale burner and 465 kW class combustion test furnace. The predicted results for the lab-scale burner by the numerical simulations were validated by the measurement results of NH radical concentration distributions obtained by Laser Induced Fluorescence. The NH-radical concentration distribution predicted by the simulation was consistent well with that measured by the experiment. Employing the same simulation method, the numerical simulation for the combustion field of 465 kW class combustion test furnace was also conducted. The numerical simulation successfully precited the tendency of the exhaust gas NO concentration reduction when the configurations of the oxidizer and fuel injection ports of the burner were changed. From the analysis of the numerical simulation data, it was found that the essential for the NO concentration reduction of the high-temperature air / ammonia / methane mixing combustion is avoiding the NO formation from ammonia

by creating the low oxygen gas composition region near the injection of ammonia gas.

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MS12-2 Spread of ammonia combustion research - Role of numerical simulation - (2)

Chair: Hisashi Nakamura
Co-Chair: Ekenechukwu Chijioke Okafor
Wednesday, May 8; 13:30 - 15:10; Room D

Detailed Diffusion Effects on Thermal and Chemical Kinetics in a Turbulent NH3/H2 Non-premixed Flame

Ahmed Abdelnasser Tawfik Adam, Reo Kai, Hiroaki Watanabe
Kyushu University, Japan

Ammonia (NH3) and hydrogen (H2), as sustainable fuel sources, may become more important in achieving and controlling zero carbon emissions from combustion devices. A thorough understanding of detailed diffusion (DD) is necessary for the proper prediction of combustion processes fueled by NH3-H2, especially because of the higher diffusivity of H2 compared with thermal diffusivity and diffusivities of O2 and NH3. Assuming that turbulent mixing greatly exceeds molecular mixing, it is common practice in turbulent combustion simulations to ignore the effects of DD, hence simplifying the modeling process. However, it is important to understand that, despite this assumption is valid for hydrocarbon fuels, it loses significance when it comes to the burning of H2 because of the significant influence of DD. In this work, two direct numerical simulations of a turbulent NH3/H2 non-premixed flame in the mixing layer are conducted, one considers the DD and the other assumes the unity Lewis number (ULN) to investigate the DD effect. It is found that the DD lets more fuel diffuse toward the flame front, which enhances the stability of the flame significantly compared with the ULN assumption.

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Modelling of turbulent premixed swirl flames for 70/30 vol% NH3/H2 fuel-air mixtures

Joanna Jójka[1], Ali Alnasif[2], Syed Mashruk[2], Agustin Valera-Medina[2]
[1]Poznan University of Technology, Poland, [2]Cardiff University, United Kingdom

Accurate prediction of ammonia turbulent combustion emissions is crucial for the further development of combustion systems. Fuel-air mixtures with a 70/30 vol% NH3/H2 ratio were numerically investigated for a premixed burner setup with a fixed power of 10kW.

RANS calculations were performed with Reynolds stress transport using a complex chemistry and species transport model with respect to thermal and mixture averaged diffusion. Turbulence-chemistry interaction was modelled using the Eddy Dissipation Concept with Stagni and Nakamura kinetic reaction mechanisms.

The numerical results were evaluated in terms of flame shape, flame stability and emissions, with a focus on the NO, N2O and NO2 shares in the flue gases and the unburned NH3 prediction capabilities of the model.

Qualitative and quantitative agreement was achieved within the equivalence ratio (φ) range of 0.8-1.2, while the relative error of the NO predictions did not exceed 3.5% with respect to the uncertainty of the experimental results. Gradients of NH3 and NO shares in the flue gases for the modelled turbulent flames were found to be shifted towards stoichiometric conditions compared to the same mixture and mechanism for a burner-stabilised stagnation 1D flame outcome. A significant overprediction of NO emission was expected for very lean mixtures φ = 0.6, as deviations can be related to the simplification of fine structure reaction fractions commonly used in the EDC model. Despite its limitations in the very lean conditions, the model correctly predicted a decrease in NO concentration in the flue gases, associated with a rapid increase in N2O emission.

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INSIGHT INTO NH3 FORMATION CHARACTERISTICS AT RICH CONDITIONS IN 70/30 VOL% NH3/H2 FLAMES

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Recent studies have highlighted that in fuel blends with a 70/30 vol% ratio of ammonia/hydrogen, the ratio of final to initial mole fractions of NH3 is notably high. This

finding underscores the importance of a comprehensive understanding of the product gases, especially the residual NH3, in NH3/H2 laminar flames. Such understanding is critical for designing NH3-fueled combustors to comply with stringent emission regulations. Understanding the underlying chemistry in the oxidation of NH3/H2 mixtures is a pivotal factor for the flexible utilization of these mixtures in various applications, including propulsion systems and power generation. In this context, the current work investigates 70 kinetic reaction mechanisms from the literature in atmospheric conditions. This study aims to evaluate the effectiveness of these mechanisms in predicting the mole fraction of unburned NH3 in a volumetric fuel mixture of 70% NH3 and 30% H2. The findings revealed that the Lamoureux kinetic model yielded reliable estimations of the unburned NH3 within the equivalence ratio (φ) range of 1-1.2. However, its accuracy decreased by around 1.4 of φ. Notable variations were observed in the reaction steps and rate parameters among these tested mechanisms. Predominantly, NH3 was converted to NH2 radicals through reactions with OH across all temperatures, with a secondary role played by O radicals at low to intermediate temperatures. At higher temperatures, NH3 dehydrogenation also occurred via H radicals, as evidenced in the NH3+H ⇌ NH2+H2 reaction. Additionally, at the combustion exit, NH3 regeneration was primarily driven by the NH3 ⇌ NH2+H reaction at a temperature of 504 K.

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Evaluation of a manifold model for lean ammonia/hydrogen/nitrogen-air laminar premixed flames

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Partially cracked ammonia is a promising hydrogen carrying fuel with logistical advantages compared to pure hydrogen. Under fuel-lean conditions, ammonia/hydrogen/nitrogen-air premixed flames can be thermodiffusively unstable. These instabilities have implications for flame propagation speeds as well as the local formation of nitrogen oxides and nitrous oxide. In this work, detailed two-dimensional simulations of laminar premixed flames are conducted to understand the development of thermodiffusive instabilities in flames of ammonia/hydrogen/nitrogen mixtures and air. The degree of ammonia cracking is varied to understand the influence of fuel composition on the instability behavior and subsequent formation of nitrogen oxides and nitrous oxide. The databases from these simulations are then used to evaluate a premixed manifold model. Manifold models significantly decrease computational cost by mapping the high dimensional thermochemical state to a lower dimensional manifold. This work assesses how accurately a manifold model for premixed combustion, including differential diffusion effects and flame curvature influences, captures differential diffusion effects as well as the formation of nitrogen oxides and nitrous oxide.

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Chemical effects of ammonia on soot suppression in laminar diffusion flames

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The co-firing of ammonia (NH3) with hydrocarbon fuels is an effective strategy for reducing CO2 emissions and addressing the inherent low reactivity of NH3. However, soot formation presents a potential challenge in this context. In this study, numerical investigations of laminar counterflow and coflow diffusion flames are conducted to understand the chemical effect of NH3 on soot formation. To improve the prediction of reduced PAH with NH3 substitution, an additional reaction of C3H3 and HCN is incorporated into the gas-phase mechanism. Moreover, a recently proposed reactive soot inception model is employed and the soot surface growth model is improved to account for the blocking of active sites on the soot surface by NH3 decomposition products (such as NH2). The results demonstrate that NH3 substitution leads to a decrease in H radical and an increase in H2. Such a chemical effect is integrated well into the reactive inception model, leading to improved predictions of soot volume fraction and mean particle diameter in NH3-blended ethylene flames. Moreover, the consideration of soot-NH2 reactions further reduces the HACA surface growth rate in NH3-blended flames, leading to an additional improvement in the predictions of the sensitivity of soot volume fraction and mean particle diameter to NH3 substitution. This study demonstrates the importance of C-N chemistry in both gas-phase and solid-gas reactions on PAHs and soot formation. Future work is needed to develop more comprehensive C-N chemical pathways for predictions of co-firing of ammonia with hydrocarbon fuels.

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MS12-3 Spread of ammonia combustion research - Role of numerical simulation - (3)

Chair: Hisashi Nakamura
Co-Chair: Ekenechukwu Chijioke Okafor
Wednesday, May 8; 15:30 - 17:10; Room D

Ammonia/coal co-firing on a complex CI-α burner with preheated combustion air streams using multi-stream FPV-LES approach

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The FPV-LES approach applied to multi stream complex burners with preheated secondary, tertiary, and staged combustion air streams, closely resembling conditions observed in commercial-scale power plant burners has limitation considering different temperatures of oxidizer streams. To address this limitation, a new approach is introduced that considers the oxidizer temperature as an additional lookup parameter by using three different non-adiabatic flamelet libraries corresponding to different oxidizer temperatures for primary, secondary, and tertiary/staged streams. The thermochemical space is parameterized using seven-dimensional non-adiabatic flamelet library, incorporating three mixture fractions for ammonia, coal volatiles, and char-off gases as well as mixture fraction variance, reaction progress variable, total enthalpy, and oxidizer temperature. The accuracy of proposed approach is tested by performing multi stream FPV-LES modeling of ammonia/coal co-firing on a 760 kWth semi-industrial test furnace of Central Research Institute of Electric Power Industry (CRIEPI) equipped with advanced low NOx CI-α burner with preheated secondary, tertiary, and staged combustion air streams. The 7D NA-FPV-LES model accurately captured the flow field in primary reaction zone, which previous model failed to do due to differences in oxidizer stream temperatures. This resulted into more accurate O2 mole fraction profile and, consequently, a better NO emission profile.

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A kinetic mechanism for ammonia-doped hydrocarbon combustion: emerging nitrogen chemistry of C3 and larger species

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Ammonia (NH3) is a hydrogen carrier that can facilitate the sustainable energy transition by enabling co-firing with hydrocarbon fuels. In this work, we developed a new kinetic mechanism for ammonia-doped hydrocarbon combustion by employing a combination of ab initio and kinetic study. New reaction pathways of large hydrocarbons reacting with NH3 and NH2 radical were proposed, and their rate constants were determined by high-level quantum chemistry calculation and robust kinetic method. After merging a C2H4 combustion mechanism with the nitrogen chemistry up to C2, these proposed pathways and recent literature on small nitrogen-containing species (e.g., NH2, NH3, and HCN) reacting with C3 and larger hydrocarbons (e.g., polycyclic aromatic hydrocarbons) were included. This mechanism was validated against literature measurements on laminar burning velocity of C2H4/NH3 premixed flames, ignition delay time of NH3/O2/Ar mixtures, and profiles of temperature and mole fractions of some gas-phase species in a set of pure, N2-doped, or NH3-doped C2H4 counterflow diffusion flames. Simulations also show that these additional pathways are important to reproduce experimentally measured quantities, such as the PAH reduction in C2H4/NH3 diffusion flames. Compared to literature mechanisms, our new kinetic model brings the model predictions closer to experimental measurements without the need for empirical adjustments.

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Investigation of temperature and species distributions in ammonia diffusion flames

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Information on radical distributions in ammonia (NH3) flames is limited but vital for the development of high-fidelity ammonia kinetic models. In this study, the temperature and NH/OH radical distributions in the counterflow NH3 diffusion flames have been investigated both experimentally and numerically. The flame temperature was varied in the range of 2200 to 2750 K by controlling the dilution ratio and measured using the Rayleigh scattering thermometry. The distributions of NH and OH were captured by planar laser-induced fluorescence (PLIF).

Furthermore, two-dimensional numerical simulations considering the actual burner configuration were performed to validate the performance of recently proposed ammonia kinetic models against the present experimental data, and additional one-dimensional numerical simulations were also conducted to obtain insights into the discrepancies among the selected ammonia models. The results show that all tested models reasonably predict the flame temperatures. Compared with the experimental data, the models predict the distribution of OH well at temperatures below 2300 K but tend to underpredict the width of OH profiles as temperatures increase. On the other hand, the models show larger discrepancies in predicting peak OH/NH concentrations at lower temperatures, which could be the focus of future refinement of ammonia kinetic models.

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Numerical simulation of laminar flame propagation of ammonia/air premixture under microgravity conditions

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Effect of gravity on laminar flame propagation of ammonia/air premixture is investigated under a normal-gravity condition and a micro-gravity condition by using the numerical simulation of a three-dimensional spherical propagating flame. In order to accurately capture the flame propagation, direct numerical simulation is applied to the flow field with a minimum grid size of 0.5 mm. And GRI-Mech 3.0 mechanism is adopted for detailed chemical reactions of ammonia/air premixture. Numerical calculation using a cubic calculation domain captures spherical flame propagation within approximately 50ms from the start of ignition of the ammonia/air premixture. The propagation speed of spherical flame propagation by numerical simulation is measured using the same flame front tracking method as in the experimental measurement and compared with the experimental values.

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Chemical kinetic studies of ammonia and their application in numerical combustion simulations

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Ammonia is now recognized as an important chemical for storing and transporting renewable energy. In recent years, ammonia combustion for energy utilization has attracted attention in order to compensate for fluctuations in electricity produced from renewable energy sources and to achieve the decarbonization of large-scale transportation and high-temperature heating processes that are difficult to electrify. This presentation introduces background, recent studies of ammonia chemical kinetics, and their application to numerical combustion simulations in our group. To improve prediction performance of detailed ammonia reaction models, species measurements in ammonia oxidation at intermediate temperatures have been conducted using a micro flow reactor with a controlled temperature profile (MFR) and gas analyzers such as a gas chromatograph and mass spectrometer. Measured results in MFR as well as literature data such as ignition delay times, laminar flame speeds, and speciation data in other systems have been used for model validation. In addition to the detailed models, small ammonia reaction models are necessary for large-scale numerical combustion simulations such as boilers and furnaces. The presentation also introduces generation method of small ammonia reaction models using genetic algorithms.

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MS13 Advances in dimensionality reduction and manifold learning for the parametrization and modeling of large combustion systems

Organizers: Temistocle Grenga[1], Alessandro Parente[2]

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MS13-1 Advances in dimensionality reduction and manifold learning for the parametrization and modeling of large combustion systems (1)

Chair: Temistocle Grenga
Co-Chair: Alessandro Parente
Friday, May 10; 13:00 - 15:00; Room H

Dynamic Mode Decomposition analysis of premixed flames

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Dynamic Mode Decomposition (DMD) has the capability to decompose flow field data into distinct coherent modes, enabling the determination of their oscillation frequencies and rates of growth or decay. This permits the exploration of unsteady and dynamic phenomena, a capability beyond what conventional statistical analyses can provide. This decomposition method is applicable for analyzing data encompassing a wide spectrum of temporal and spatial scales because it identifies structures characterizing the physical phenomena independently of their energy content.

In this study, a specially designed DMD algorithm tailored for handling massive databases is utilized to examine three-dimensional Direct Numerical Simulation data of spatially evolving turbulent planar premixed methane/air jet flames across different Reynolds numbers.

This study aims to identify the key modes and frequencies crucial for the evolution of the flow field, particularly concerning physical phenomena such as heat release and turbulence and their interaction.

The results are compared to previous analyses of hydrogen/air jet flames in order to assess the role of differential diffusion in both fuel/air mixtures considered, as well as their impact with respect to the turbulence intensity.

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Vector Quantization Partial Least Square (VQPLS) for enhanced semi-supervised clustering for combustion manifold regression

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PCA-based combustion simulations are increasingly being used through the development of PC-transport approaches. In such models, the tabulation of the source term of new variables (PC scores) is a fundamental step and is often approximated by complex nonlinear functions, such as Artificial Neural Networks (ANN) or Gaussian Process Regression (GPR). However, the training of these models can be computationally expensive, and their functional forms may introduce non-negligible overhead costs during simulations.

To address this challenge, the presented clustering algorithm aims to identify data clusters where the relationship between PCA scores and the source term can be effectively approximated by a linear model. The algorithm relies on Partial Least Squares (PLS), a dimensionality reduction technique that considers the relationship between the independent and dependent variables. This is particularly attractive to partition thermo-chemical state-space effectively according to their relationship with the source term. Therefore, in such a routine, the data are clustered to minimize local linear regression errors. A user-defined threshold on the desired error is then fixed, and clusters with linear regression error above such threshold are joined and modelled with nonlinear tools. This work will be beneficial in reducing training time of complex nonlinear tools, as well as simplifying their functional form.

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Application of In-Situ Adaptive Manifolds (ISAM) for the study of highly stratified multi-regime flames

Anurag Surapaneni
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The triple flame represents a canonical combustion problem and serves as a benchmark test case for studying multi-regime combustion models. In this current investigation, triple flames at different mixing lengths are examined using finite rate chemistry, tabulated manifolds based on premixed flamelets, and a multi-modal combustion model. The finite rate chemistry method is employed as a reference to assess both the tabulated premixed flamelet manifold and the multi-modal combustion models. The study's objective is to quantify deviations and identify limitations in the application of manifold-based methods in multi-regime problems. Manifolds with varying resolutions are utilised in both tabulated methods to assess the impact of manifold resolution on the solutions. Key aspects of the problem, such as flame shape, flame surface area, and propagation speed, are compared across the different methods. The study then proceeds to a scatter plot analysis of the thermochemical states obtained from these methods. It concludes by delineating the limitations within which manifold methods can be effectively applied. Finally, the scope for future work is outlined.

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On-the-fly reduced-order modeling of large combustion systems leveraging time-dependent bases with CUR decomposition

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While data-driven reduced-order modeling (ROMs) have been successfully demonstrated in turbulent combustion simulations, their performance often relies on the selection and availability of appropriate datasets for offline training. Recently, ROM leveraging time-dependent bases with CUR decomposition, called TDB-CUR, was introduced to approximate the solution of nonlinear matrix partial differential equations by adapting the reduced-order model on-the-fly without relying on a priori knowledge, demonstrating the accuracy, robustness, and efficiency of the model for a range of non-linear problems. In this presentation, the applicability of the TDB-CUR is assessed for chemically reactive flow simulations. A clustered dynamic adaptive chemistry and rank-adaptive scheme are coupled with TDB-CUR to enhance the computational efficiency of the ROM. It has been successfully demonstrated that TDB-CUR has an excellent agreement with direct numerical simulation (DNS) results for methane-air flames for various canonical configurations. The performance of the TDB-CUR approach is further evaluated using DNS of compression ignition of large hydrocarbon fuels in the negative temperature coefficient regime. The results show that TDB-CUR can accurately replicate multi-stage ignition of a primary reference fuel/air mixture under engine relevant conditions.

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Understanding the role of latent variables in accelerated integration of stiff chemical systems using autoencoders

Vijayamanikandan Vijayarangan, Harshavardhana A Uranakara, Francisco E Hernández Pérez, Hong G Im
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Efficient computation of finite-rate chemical kinetics remains a critical challenge in modern reacting flow simulations due to inherent system stiffness. Building upon our previous research, this study introduces a dynamic-informed data-driven methodology aimed at mitigating stiffness in chemical dynamics. By leveraging a combined autoencoder and neural ordinary differential equation approach, this method effectively eliminates stiffness, thereby relaxing the time step requirements. The autoencoder facilitates the computation of an optimized low-dimensional latent space, yet its formulation remains to be explored. Due to this, the combined neural system is treated as a black box. Recognizing the latent space as a curved manifold with curvilinear coordinates, simple tools from Riemann geometry are employed for the analysis. In this work, information geometry is utilized to unveil the geometric structure of the latent variables corresponding to the physical state variables within the statistical model. This exploration delves into revealing insights about the shape and geometry of the manifold. Additionally, the necessary degrees of freedom essential for describing the chemical dynamics accurately are determined. The findings contribute to a deeper understanding of the underlying structure, aiding in more efficient computational modelling of reacting flow systems.

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Effect of Parametric Uncertainty in Numerical Simulations Using Dimensionality Reduction and Non-linear Regression: Application to a Hydrogen-Fueled Flameless Combustion Furnace

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This work explores cost-effective uncertainty quantification (UQ) methods, crucial when dealing with high-dimensional uncertain parameter spaces. Employing proper orthogonal decomposition and gaussian process regression (POD/GPR) technique, we constructed a surrogate model for a 2-dimensional RANS response involving nine uncertain parameters encompassing reaction rates, turbulence, combustion models, and inlet mass flow variations. The surrogate model provided insights into the variance contributions of these parameters.

Notably, within the furnace's flame region, the turbulence parameter $C_{2\varepsilon}$ and the PaSR combustion model constant C_{mix} exhibited significant influence on response variability. Conversely, farther from the flame, uncertainty in the inlet air mass flow u_{air} gained prominence due to its substantial impact on the combustion chamber's recirculation pattern driven by the air inlet jet.

More in general, the POD/GPR approach's efficacy lies in navigating complex spaces with minimal simulations compared to traditional UQ methods. This enables an initial assessment of numerous uncertain parameters in simpler models like 2D RANS. Then, the more critical parameters can be scrutinized using advanced models like 3D RANS or LES.

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MS13-2 Advances in dimensionality reduction and manifold learning for the parametrization and modeling of large combustion systems (2)

Chair: Temistocle Grenga
Co-Chair: Alessandro Parente
Friday, May 10; 15:20 - 17:00; Room H

Generalized progress variable and cross-dissipation rate in turbulent lifted flames using a multi-modal manifold-based combustion model

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Multi-modal manifold models in mixture fraction and generalized progress variable have been previously implemented in Large Eddy Simulation (LES), demonstrating that manifold-based models can be generalized to no longer require a priori assumptions about the underlying combustion process. In this work, the influence of the definition of the generalized progress variable and its influence on the cross-dissipation rate of the mixture fraction and the generalized progress variable is investigated with LES of a multi-modal turbulent lifted hydrogen jet flame in a vitiated coflow. The multi-modal manifold-based model is implemented within the In-Situ Adaptive Manifolds (ISAM) computational framework, and two definitions of the generalized progress variable are considered: a standard linear generalized progress variable that is a normalized product mass fraction and a nonlinear generalized progress variable whose gradients vanish in the asymptotic limit of nonpremixed combustion. This aspect of the generalized progress variable definitions significantly alters the relative magnitudes of the mixture fraction and generalized progress variable dissipation rates and fundamentally changes the behavior of the cross-dissipation rate.

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Dynamic Cell Clustering with Principal Component Analysis for massively parallel multi-regime reactive flows

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Dynamic Cell Clustering (DCC), also referred as Cell Agglomeration, is an optimisation technique used to reduce the cost of finite-rate chemistry in reactive flows. It consists of three steps: i) grouping of elements with similar composition into clusters, ii) computation of a single element per cluster and iii) mapping of the computed elements to the remaining elements of the cluster through interpolation and extrapolation. Principal Component Analysis (PCA) is used during the initial clustering step to identify dominant features within the composition space and reduce its dimensionality. This approach is demonstrated in the CORIA Rouen Spray Burner (CRSB) using either global parallel PCA and local PCA within each core. In this burner, multi-regime combustion occurs through fuel droplets that evaporate before and within the flame front leading to partially premixed and diffusion flames, making it a challenging case for PCA. The simulations run on 10,000 cores with 300 million tetrahedral cells. With the DCC-PCA methodology, the cost of chemistry is reduced by 50% while introducing a relative error on source terms of less than 1%.

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JuLES: A Data-Driven Framework for Subfilter Model Development of Reactive Flows on Supercomputers at Scale

Mathis Bode

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JuLES (JUelich Large-Eddy Simulation) is a disruptive Software-as-a-Service (SaaS) platform for developing reduced models of reactive flows in the shortest possible time and with unprecedented predictive accuracy. It is integrated into the supercomputing environment at the Jülich Supercomputing Centre, including the JupyterLab cloud, HPC resources, and quantum computing, to provide maximum opportunities with minimum barriers to entry. Technically, JuLES uses Physics-Informed Enhanced Super-Resolution Generative Adversarial Networks (PIESRGAN) for Large-Eddy Simulation (LES). PIESRGAN for LES enables the data-driven development of reduced models for reactive flows that have been shown to be significantly superior to existing models in terms of prediction accuracy, robustness, and universality, while reducing simulation costs by two orders of magnitude and I/O by as much as three orders of magnitude. Consequently, industrial development processes are potentially accelerated by years. The combination of classical, well-established fluid mechanics techniques and cutting-edge AI technology, its ability to fully scale on today's supercomputers, and its cloud-based n:m on-the-fly training make it a very powerful tool for industrial transformation and even ready for the upcoming exascale machine JUPITER. Multiple combustion applications are discussed in this work.

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A Co-kurtosis PCA based Dimensionality Reduction for Chemical Kinetics: A-Posteriori Analysis

Shiva Sai Tadikonda[1], Hemanth Kolla[2], **Aditya Konduri**[1]

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A low-dimensional representation of thermo-chemical scalars based on cokutorsis principal component analysis (CoK-PCA) has been shown to effectively capture stiff chemical dynamics in reacting flows relative to the widely used principal component analysis (PCA). The effectiveness of the reduced manifold was evaluated in a priori analyses using both linear and nonlinear reconstructions of thermo-chemical scalars from aggressively truncated principal components. In this study, we demonstrate the efficacy of a CoK-PCA-based reduced manifold using a posteriori analysis. Simulations of spontaneous ignition in a homogeneous reactor that pose a challenge in accurately capturing the ignition delay time as well as the profiles of the scalar within the reaction zone are considered. A manifold assessment in the a priori setting showed that PCs from CoK-PCA are less stiff than those from PCA. The principal components were evolved from the initial conditions using two ODE solvers. First, a standard solver that uses an aritifical neural network to estimate the source terms. Second, a neural ODE solver that incorporates the time integration of PCs in training ANNs, which predict their source terms. The time-evolved profiles of the PCs and ANN-reconstructed thermo-chemical scalars demonstrate the robustness of the CoK-PCA based low-dimensional manifold in accurately capturing the ignition process. Furthermore, we observed that the neural ODE solver provides more accurate results than the standard ODE solver. The results from this study demonstrate the potential of CoK-PCA-based manifolds to be implemented in massively parallel reacting flow solvers.

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Effects of combustor wall temperature on the low-temperature chemistry in turbulent premixed DME/air swirl flames

Wenjun Lin[1], Zhenhua An[2], Weijie Zhang[1], Jinhua Wang[1], Zuohua Huang[1], Huangwei Zhang[3]

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The environment of the outer recirculation zone (ORZ) in swirl flame is favorable for low-temperature ignition under fuel lean conditions, but the factors affecting the ORZ combustion modes remain unclear. This study investigates the effects of wall thermal boundary conditions on combustion modes using the LES-FGM method. The results of tabulated chemistry were firstly validated by the experiment data and the detailed chemistry. It is found that the flame topology is highly sensitive to the wall thermal boundary condition. Based on the correlation between temperature and species in the time-averaged results, it is inferred that there is a link between wall temperature and combustion modes. Through temporal analysis of species and heat release rate in the ORZ, the stable Mode II and Mode IV as well as the unstable Mode III are identified. Subsequent chemical reaction pathway analysis on specific probes reveals that different combustion modes undergo distinct chemical reaction pathways. Finally, the definition of combustion modes used in experiments is refined by utilizing the chemical reaction fluxes in the simulations. This refined definition is applied to classify combustion modes across the entire computational domain. The results confirm the consistency between the combustion modes determined in experiments based on OH and CH2O and those determined in simulations using chemical reaction fluxes. Based on these findings, the adaptability of the FGM-LES method in predicting lean premixed swirling flame can be ascertained, and the mechanism of wall thermal boundary conditions on combustion modes in premixed swirling flame is recognized.

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MS14 Numerical modeling and simulation of reactive dense particle-laden flows

Organizer : Takuya Tsuji
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MS14-1 Numerical modeling and simulation of reactive dense particle-laden flows (1)

Chair: Takuya Tsuji
Wednesday, May 8; 10:40 - 12:20; Room G

A new DEM-CFD solver for reactive dense gas-solid flows based on a characteristic splitting

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Reactive dense gas-solid flows play important roles in carbon neutrality. Interplays between flow and dense particle dynamics, heat and mass transfers, and chemical reactions over a wide range of spatiotemporal scales make its behavior complex. Due to its inherent opacity, experimental diagnosis is difficult, and the realization of high-fidelity numerical simulation is important but still challenging. In this study, a new unresolved DEM-CFD solver based on the fractional-step method is proposed. A characteristic splitting enables the separation of the acoustics from the advection, resulting in the efficient calculation of gas motions. All governing equations including the Helmholtz equation for the pressure variations are volume-averaged. Details of the algorithm and the results of several validation cases are presented.

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Multi-scale simulation of solid fuel conversion in dense particulate reactive systems

Shuai Wang, Jiahui Yu, Junjie Lin, Kun Luo, Jianren Fan
Zhejiang University, China

Solid fuel conversion is quite common in many engineering fields, including biomass gasification, coal combustion, solar panel waste pyrolysis, chemical looping combustion, blast furnace ironmaking, etc [1]. These kinds of processes are extremely complex involving both physical changes and chemical changes. Understanding the fundamentals governing the gas-solid flow and coupled heat and mass transfer is of paramount importance to the design, control, and optimization of dense particulate reactive systems. In this talk, we will present the recent work related to the development of multi-scale numerical methods, including computational fluid dynamics-discrete element method (CFD-DEM), coarse-grained method (CGM), and multiphase particle-in-cell (MP-PIC) with complex thermochemical sub-models [2-4]. The integrated models were validated using experimental data, demonstrating their reasonable accuracy.

The CFD-DEM model enables the high-fidelity simulation of lab-scale apparatuses and provides detailed information on particle residence time, heat transfer contribution, carbon conversion ratio, and other crucial parameters. In contrast, the CGM and MP-PIC models facilitate the high-efficiency simulation of pilot-scale and industrial-scale apparatuses, offering in-depth insights into vital in-furnace phenomena such as cluster evolution, size-/density-induced segregation, gas pollutant formation, and so on. The multi-scale simulation approach is expected to provide valuable information for optimizing the process of solid fuel conversion in reaction-intensive apparatuses.

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Particle-resolved lattice Boltzmann simulations for sedimentation of reactive particles involving coke deposition

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Catalysts have been widely applied in various chemical processes. When hydrocarbons are employed as feedstock, coke deposition on the catalyst can result in the coverage of active sites and blockage of nanopores, leading to the decrease of reaction rates and even deactivation of the catalyst1,2. In this work, a particle-resolved lattice Boltzmann method (LBM) with a hybrid multiple-relaxation-time scheme was used to investigate the effect of coke formation on particle-fluid interaction. The particle-fluid interface was treated using the Immersed Boundary method (IBM). The sedimentation of a single particle and a pair of particles with varying reaction rates constant have been simulated, in which the change of catalyst physical property and reaction activity due to coke deposition were considered. The results show that the increase of coke deposition on the catalyst can accelerate the sedimentation rate of a single catalyst particle owing to the gradual increase of weight. For the case of a pair of particles, the drafting, kissing, and tumbling (DKT) phenomenon of coked particles is different from that of non-reactive particles. Suppose that these two particles have different deactivation rates because of uneven concentration distribution, and the second DKT phenomenon occurred earlier with a larger reaction rate.

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Coarse grained CFD-DEM simulations of iron-iron oxide conversion in fluidized beds

Yali Tang, Niels Gerbrand Deen
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Iron powder has enormous potential to boost the energy transition, as an energy carrier in a carbon-neutral circular energy economy. This is realized by the cyclic storage and release of renewable energy via processes of iron reduction and oxidation.

In this work, a numerical model, coupled between CFD and coarse-grained DEM, is developed for simulating chemical conversion processes of micron-sized iron/iron oxide powder in fluidized beds (FB) at intermediate temperatures. An unreacted shrink core model is incorporated for iron reduction/oxidation, utilizing reaction kinetics from thermogravimetric analysis experiments. Furthermore, the temperature-dependent solid bridge force is considered as the interparticle cohesive force. With careful validation, the developed model is demonstrated to predict quantitatively the effects of different operating parameters (such as temperature, gas velocity, reactive gas concentration) on the oxidation/reduction behaviour of iron/iron oxide powder. The temperature is found crucial to both oxidation and reduction processes. Increasing temperature, on one hand, speeds up the chemical reaction. On the other hand, higher temperature triggers the sintering of solid particles, which may cause serious agglomeration or even defluidization. An optimal operating temperature window has been determined from systematic simulations of bubbling FB. Finally, simulations considering different reactor types (bubbling FB, turbulent FB, spouted FB, vibrating FB) provide design guidance to the engineering processes of the iron power technology.

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Numerical modelling the reaction propagation in Al based thermites

Emilian Tichtchenko, Alain Esteve, Benoit Bedat, Olivier Simonin, **Carole Rossi**
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Nanothermites are promising energetic materials as their high-temperature reaction driven by the oxidation of a metallic fuel associated with the reduction of an oxidizer, can exhibit extremely fast burning rates, exceeding hundreds of m/s. By modifying reactant size, stoichiometry, and compaction conditions, it is possible to tailor combustion properties, including temperature and intermediate reactions. Unfortunately, the complex multiphasic physics governing thermite combustion, where combustion gases interact with burning particles, is still poorly understood and documented, while being the key step to depict the dynamics of the flame front. We developed a first one-dimensional (1D) model that describes the dynamics of the reaction front propagation in Al/CuO powdered thermite considering the reacting flow combined with heat transfer, chemistry and fluid flow. CuO was chosen as it is the widest used metallic oxidizer, that decomposes below the flame temperature, leading a a gas phase reaction. Separate mass, momentum and energy transport equations for the three phases, namely Al, CuO particles and gas mixture, are written in the frame of N-Euler approach for multiphase reactive flows. These equations are coupled by modeled interphase transfer terms. After the description of the theoretical formulation and numerical method, two numerical experiments, i.e. mixture of Al/CuO powder burning into semi-open and closed tubes, will be discussed with the goal to understand the multiphase flow physics in the

thermite flame front.

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MS14-2 Numerical modeling and simulation of reactive dense particle-laden flows (2)

Chair: Yali Tang
Wednesday, May 8; 13:30 - 15:10; Room G

DEM-CFD modeling of limestones with actual diameter distribution flowing down in a combustion field in a rotary kiln

Susumu Tsuchiya[1], Masaya Muto[2], Fumiteru Akamatsu[3], Ryoichi Kurose[4], Yuta Umeno[5], Takayuki Nishiie[5]
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In this study, is to clarify the gas temperature distribution in the kiln and the behavior of limestones flowing down in the kiln by performing a numerical simulation of the combustion field in the actual rotary kiln.

RANS simulation coupled with Discrete Element Method (DEM) is applied to a combustion reaction flow field with limestone motion in a real rotary kiln. The governing equations for the gas phase are the conservation equations of mass, momentum, energy, mass of each chemical species. Standard k-epsilon model is used as a turbulent model. For the flowing limestone, the Discrete Element Method (DEM) is applied to consider the contact force between the limestone and the inner wall of the kiln, and between the limestone particles. A limestone particle size distribution based on measured values in the actual kiln is given as the limestone injection condition in the simulation.

Result shows that the present analysis satisfactorily predicts the gas chemical composition at the outlet of kiln, and that the mutual interference and decarboxylation process of limestone are well reproduced.

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Consistent treatment of added mass, and mass and heat exchange in dense reactive gas-particle flow simulations

Rodney O Fox[1], Jacob Posey[2], Ryan W Houim[2]
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In recent work, we have developed a multifluid model for high-speed, polydisperse, gas-particle flow with solid and gas-phase reactions. This model is well-posed due to the inclusion of added mass and the particle-fluid-particle stresses. The added mass is modeled as fluid surrounding a solid particle and traveling with the same velocity as the particle. In the context of non-reacting flow without mass transfer, the volume of fluid representing the added mass changes locally in a dense flow to adjust to the local volume fraction of the disperse phase. Moreover, the added-mass fluid and the solid particle are assumed to have the same temperature, which can be different than the continuous gas phase moving with its own velocity. In this work, we extend the model in a consistent manner to allow for the added-mass fluid and the solid to have different thermodynamic properties, which are also different than the continuous gas phase. For reactive flows, the chemical mass fractions in the solid, added-mass fluid and continuous fluid will generally be different and must be modeled consistently to obtain the correct overall mass/heat-transfer rates. Here, dense reactive gas-solid flow simulations for high-speed flows are used to verify the proposed model under different flow regimes with and without chemical reactions.

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Multi-scale insights of chemical looping combustion in a three-dimensional bubbling fluidized bed

Junjie Lin, Kun Luo, Jianren Fan
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Chemical looping combustion (CLC) has emerged as an effective carbon capture and storage (CCS) technique. Yet, the intricate interaction of flow, temperature, and species fields presents challenges in comprehending the underlying mechanism from multi-scale aspects. In this work, a computational fluid dynamics-discrete element method (CFD-DEM) reactive model is developed, featuring a coarse-grained method to provide efficient calculation and a modified drag model to consider the polydispersity effect. After comprehensive validations, the integrated model is applied to simulate the CH4-fueled CLC process in a fuel reactor (FR), with a discussion of the effects of particle size distribution and reactor inner diameter on

the system performance. The results demonstrate that the particle-scale polydispersity, bubble-scale dynamics, and reactor-scale structure can significantly influence the interactions between gaseous fuel and oxygen carriers in the CLC system. These factors play a crucial role in determining the thermochemical characteristics of the system. Particularly, bubbles in the FR with a smaller diameter display a characteristic of "fewer but larger", whereas bubbles in the newly devised FR with a larger diameter exhibit a feature of "more but smaller". Consequently, enhanced uniformity in gas-solid physicochemical properties, heightened CO2 concentration, and improved combustion efficiency can be achieved in our newly designed CLC reactor. Overall, this study imparts valuable multi-scale insights into the physical-thermal-chemical characteristics of the CLC process.

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Full-loop reactive simulation of catalytic cracking CFB system with mechanical valves

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Circulating fluidized bed (CFB) systems are the core units of many chemical and energy processes. In this study, a full-loop simulation of an industrial reaction-regeneration CFB system is realized by modeling mechanical valves under the framework of two-fluid model. The EMMS-matrix model is used for regions operated in fast fluidization or pneumatic transport, and the EMMS-bubbling model for the bubbling or turbulent fluidization. The twelve-lump kinetic model is used to describe endothermic catalytic cracking reaction, and the coke combustion model is adopted for exothermic coke burning reaction. The solid phase is treated as a mixture of solid catalysts and coke, and the gas phase is treated a mixture of twelve species (eleven is gas products and the other is steam). During the circulation of solid phase throughout the full-loop system, coke deposition on solid catalysts varies and simultaneously accompanies with heat transfer between the reactor and regenerator. The results show that compared to the full-loop hydrodynamic simulation, the reactive simulation needs much more time to achieve the loop balance, as spent solid catalysts in the regeneration part has experienced multiple circulations from the top region to the bottom region through external circulation pipe to maintain enough long residence time for complete coke burning. In addition, it is found that there exists one-order-magnitude difference in solid concentration fluctuation frequency for the full-loop simulation and the single riser simulation. Such difference should be taken into account in optimize and scale-up the mesoscale structures.

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Modelling of gas-solid reacting flows and industry applications

Yansong Shen
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Process design and control play a significant role in modern industries. Most processes and reactors are very complex, as they usually involve not only multiphase flows but also heat and mass transfers related to chemical reactions and their interactions – the so-called reacting flow where powder plays an important role in operation stability and efficiency. The operation must be optimized in order to be competitive and sustainable, particularly under more and more demanding economic and environmental conditions. This will need continuous innovative research and development. Computer simulation and modelling, supported by online data and experiments, have emerged as an indispensable adjunct to the traditional modes of investigation for the design, control and optimization of processes, reactors, and devices. Several case studies including hydrogen generation, storage and use in the net zero steel industry are presented in this talk to demonstrate that the modelling works are indeed helpful to understand fundamentals and optimize & develop new, cleaner and more efficient technologies towards net zero industry innovations with measurable outcomes and profits.

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MS14-3 Numerical modeling and simulation of reactive dense particle-laden flows (3)

Chair: Yansong Shen
Wednesday, May 8; 15:30 - 16:50; Room G

A high-order quadrature method of moments implementation for dense polydisperse granular reactive flows

Jacob Posey[1], Rodney Fox[2], **Ryan Houim**[1]
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Dense, high-speed, and reactive multiphase flow models are common in nature are routinely used in engineering applications including pyroclastic flows, heterogeneous explosive charges, and dust explosions. We recently developed a theoretical model that accounts for dense

polydisperse granular mixtures interacting with compressible reactive gases using quadrature method of moments (QMOM). Our original implementation used first-order numerical methods for 1D applications. Here, we present an extension of the method to multiple dimensions and high-order methods. The numerical fluxes for the gas and particle system are computed by approximating the full Riemann problem as a series of individual Riemann problems for the gas and each particle moment. The gas-phase fluxes are computed using a traditional approach based on the HLLC Riemann solver and fifth-order MUSCL. The Wheeler algorithm is used to convert particle moment equations into size-conditioned mass, momentum, and energy equations. The granular fluxes for each of these size-conditioned moments are computed independently and using the AUSM+-up flux scheme. The results of these individual gas and granular Riemann problems are assembled to form the transport operators of the governing equations. Effects of drag, convective heat transfer, particle collisions, etc. are integrated using an operator splitting approach with analytical approximations when possible. Results of the high-order method show substantial improvement over the first-order method. Simulations of shock waves interacting with bi-disperse aluminum particle curtains and the explosive dispersal of aluminum particles will be presented.

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GPU-accelerated CFD-DEM modeling of dense gas-solid reacting flow

Jiahui Yu, Shuai Wang, Kun Luo, Jianren Fan
Zhejiang university, China

Dense gas-solid reacting flow is quite common in many engineering fields such as energy conversion, petro-chemical processing, mineral processing, chemical engineering, and pharmaceutical manufacturing. These kinds of processes are extremely complex involving both physical changes and chemical changes. Understanding the fundamentals governing the gas-solid flow and coupled heat and mass transfer is of paramount importance to the design, control, and optimization of dense gas-solid reacting systems of various types. Computational fluid dynamics – discrete element method (CFD-DEM) has been recognized as a useful tool to achieve this goal, yet this method suffers from expensive computational resources. Accordingly, this work develops a graphics processing unit (GPU)-accelerated CFD-DEM reactive model, featuring heat transfer, heterogeneous reactions, and homogenous reactions. The accuracy of the GPU-accelerated heat and mass transfer sub-models are detailly verified and the simulation results are in good agreement with analytic solutions. Additionally, this model can accurately predict the thermochemical behavior of the particle cooling process in a bubbling fluidized bed and the coal-fueled chemical looping gasification process, confirming its reliability in simulating dense gas-solid reacting systems. Furthermore, the GPU-accelerated strategy is demonstrated to perform great speed-up performance and stability. This work is expected to provide a reliable and high-performance parallel calculation method for numerically studying the gas-solid dense reacting flows.

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A hybrid inversion model using measurement data for optimized CFD simulations of fluidized beds

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The hydrodynamic behavior in gas-solid fluidized beds is complex and the mechanism is not yet complete. The computational fluid dynamic (CFD)-based simulation models contain simplified theoretical models and empirical formulas, which may result in differences between simulations and actual situations. Here, a cross-platform hybrid model was constructed to optimize the selectable parameters of simulation models according to the measurements. The hybrid model utilized the open-source MFiX software for CFD simulation and developed in-home code for parameter optimization. And a python component was built for data transfer and runtime control between simulation and parameter optimization. The proposed hybrid model was validated by a CFD-DEM (discrete element method) simulation of a pseudo two-dimensional fluidized bed. Select the solid volume fraction at the cross-section of one static bed height as the monitoring variable (or reference) and the Kalman filtering method as the optimization algorithm. The proposed hybrid model can predict the simulated solid volume fraction change curves with dozens of time steps of simulation results, compare the predicted results with reference data, and iteratively optimize CFD parameters under an inverse strategy. The optimized CFD-DEM model can better match the reference data.

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Numerical study on unsteady combustion in Stoker furnace

Takashi Ikeda, Kenji Yamamoto, Toshihiko Setoguchi, Junji Imada
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Garbage is regarded as one of the primary carbon neutral energy resource. Waste incinerator with stoker furnace generates power using garbage, and it has relatively stable supply of electricity compared to other renewable energy resource.

In stoker furnace, energy and chemical transportation by solid phase and gas phase with chemical reaction significantly may affect the combustion phenomena. Therefore, it is necessary to construct the simulation code to consider not only solid and gas phase behavior but also interaction of each other and chemical reaction.

In this study, Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) were strongly coupled for reconstructing phenomena in stoker furnace. In addition, chemical reaction of solid and gas phase was also implemented in those simulation. Although simulation showed a similar flame location compared to actual furnace under steady operation conditions, flame had unsteady flickering. It is considered that flickering of flame mainly caused by variation of amount of intermittent fuel supply.

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MS15 Combustion simulation acceleration using GPU and manycore heterogenous computing hardwares

Organizers: Zhi X. Chen[1], Hong Im[2], Venkat Raman[3]

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MS15 Combustion simulation acceleration using GPU and manycore heterogenous computing hardwares

Chair: Zhi X. Chen
Co-Chair: Hong G Im
Wednesday, May 8; 13:30 - 15:10; Room J

GPU-accelerated CSP solver for high-fidelity simulations of reactive flows

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In this work, recent progress in the development of a Computational Singular Perturbation (CSP) solver, accelerated with Graphics Processing Units (GPUs), is presented in the context of multidimensional reacting flow simulations. An assessment of its impact on the performance of the KAUST Adaptive Reactive Flows Solver (KARFS) for high-fidelity simulations is conducted. We implemented a batched CSP solver, following the Kokkos programming model for performance portability. At each grid point, applying the operator-splitting technique, the CSP solver removes the stiffness on-the-fly and numerically integrates a non-stiff reduced order model (ROM) of the chemical kinetics operator. This permits to advance the thermo-chemical state with an explicit numerical scheme making use of larger integration time steps. On the hardware side, the solver is accelerated with GPU cards, executing the algorithm independently at each grid point and exploiting all the parallelism layers offered by Kokkos.

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nekCRF: An exascale-ready finite-rate-chemistry solver designed for GPU-accelerated supercomputers

Mathis Bode[1], Ananias Tomboulides[2], Christos Frouzakis[3]

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Most of the performance of the latest generation of HPC systems, and especially all exascale supercomputers, is based on GPUs. Many codes were originally designed to run on CPUs, and switching to GPUs is highly non-trivial. This is especially true for reactive flow solvers due to the large number of scalar fields and the resulting stiff systems. In the frame of the Center of Excellence in Combustion (CoEC), the development of nekCRF, a GPU-based solver for extreme-scale computational fluid dynamics (CFD) for low Mach number compressible reactive flows has been enabled. nekCRF is based on the well-established high-order spectral element code nekRS and solves the low-Mach form of the Navier-Stokes equations together with the energy and species transport equations. nekCRF was run on up to 3600 NVIDIA A100 GPUs of JUWELS Booster, the fastest German supercomputer, and showed excellent scaling. Single node performance was demonstrated to be very efficient due to code design and high-performance computing (HPC) optimizations. Several test cases, ranging from canonical tests and flame kernels in confined geometries to complex applications with moving meshes, confirmed the numerical and physical accuracy of nekCRF. Overall, nekCRF is fully exascale-ready and can be used to accurately simulate turbulent flames in open or closed domains with unprecedented resolution.

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An integrated framework for accelerating reactive flow simulation using GPU and machine learning models

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Recent progress in artificial intelligence (AI) and high-performance computing (HPC) have brought potentially game-changing opportunities in accelerating reactive flow simulations. In this study, we introduce an open-source computational fluid dynamics (CFD) framework that integrates the strengths of machine learning (ML) and graphics processing unit (GPU) to demonstrate their combined capability. Within this framework, all computational operations are solely executed on GPU, including ML-accelerated chemistry integration, fully-implicit solving of PDEs, and computation of thermal and transport properties, thereby eliminating the CPU-GPU memory copy overhead. Optimisations both within the kernel functions and during the kernel launch process are conducted to enhance computational performance. Strategies such as static data reorganisation and dynamic data allocation are adopted to reduce the GPU memory footprint. The computational performance is evaluated in two turbulent flame benchmarks using quasi-DNS and LES modelling, respectively. Remarkably, while maintaining a similar level of accuracy to the conventional CPU/CVODE-based solver, the GPU/ML-accelerated approach shows an overall speedup of over two orders of magnitude for both cases. This result highlights that high-fidelity turbulent combustion simulation with finite-rate chemistry that requires normally hundreds of CPUs can now be performed on portable devices such as laptops with a medium-end GPU.

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A combustion simulation program library accelerated by GPU

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This article introduces a GPU-accelerated chemical ordinary differential equations (ODE) solver library, which encompasses four primary components: the calculation of thermodynamic properties, the solution of chemical reaction rates, the calculation of Jacobian matrices for chemical reaction equations, and the solution of ODE for chemical reactions. This program library can be seamlessly integrated with OpenFoam to enhance the numerical simulation process of combustion under ideal gas conditions. Depending on the circumstances, it can boost the combustion simulation speed of OpenFoam by a factor of 10 to 100. Additionally, the program offers interfaces in both C language and Python, making it effortlessly callable by other numerical simulation programs to incorporate combustion simulation capabilities.

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Deep learning-enabled exascale flame simulation with detailed chemical kinetics accuracy on New Sunway Supercomputer

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Combustion simulation based on accurate chemical reactions is the de facto standard in simulation of ignition, engine design, etc. OpenFOAM and DeepFlame combine to implement Deep learning-enabled flame simulation with detailed chemical kinetics accuracy. The new Sunway supercomputer is an exascale heterogeneous many-core supercomputer with more than 42 million heterogeneous cores. In this work, we further enhanced the performance of the OpenFOAM and DeepFlame code on the new Sunway supercomputer through optimization in three key areas: DNN inference, sparse solver, and startup process. In the DNN inference process, we leveraged mixed precision techniques to significantly enhance the speed of DNN inference. For the sparse solver, we tailored various sparse matrix operators including SymSpMV, SpMV, SymGS, etc. based on Sunway's architecture, which greatly accelerated the construction and solution process of sparse matrices in OpenFOAM. Addressing the challenge of prolonged startup times in large-scale OpenFOAM simulations, we introduced methods such as Multi-Procedure Fusion, Foam File Indexing, and Two-Level Parallel IO. These innovations resulted in a substantial acceleration of the OpenFOAM startup process, enabling us to conduct exascale flame simulations on the new Sunway.

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MS16 High-fidelity numerical simulations using FUGAKU-scale supercomputers in Academic-Industrial Collaborations

Organizers: Kenji Yamamoto[1], Nobuyuki Oshima[2], Ryoichi Kurose[3]

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MS16 High-fidelity numerical simulations using FUGAKU-scale supercomputers in Academic-Industrial Collaborations

Chair: Kenji Yamamoto
Co-Chair: Nobuyuki Oshima
Thursday, May 9; 09:50 - 12:10; Room H

Development of High-fidelity numerical simulations for aviation and powerplant gasturbune combustors

Nobuyuki Oshima[1], Ryoichi Kurose[2], Takeo Oda[3], Tomoko Tsuru[3]

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Prediction of complex behavior of turbulent combustion flow in the gasturbine combustor has been a major industrial target of high-performance computing challenge. During these two decades, computer power development enables to perform thousand time larger of grid resolution (around 10 million to 100 billion grids) to simulate the combustors of industrial gasturbine. For this purpose, collaboration researches by using the super-computers as “Earth simulator”, “K” and “Fugaku” have developed the high-fidelity numerical simulation of turbulent combustion flows. They have investigated numerical models of large eddy simulation (LES) and flamelet approach, and also validated them for aviation and powerplant gasturbine combustors by the implementation to high-performance computing software as “Frontflow/red” and “CUBE” specially designed for the latest supercomputer in 2000’s and 2020’s, respectively. High-resolution LES has revealed turbulent mixing behavior and flame holding mechanism in the detail design of industrial combustors. Prediction of NOx production under lean turbulent combustion are well developed by the high-fidelity solution of instantaneous profiles of temperature and fuel mixture. Carbon less fuel as hydrogen mixing and liquid fuel including spray behavior for aviation engine are most recent challenges towards a full simulation of gasturbine combustors.

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Evaluation of Ignition Feasibility in an Aviation Engine: Preliminary Equivalence Ratio Results and Ongoing Developments in FUGAKU-Enabled, BCM-Based Large-Eddy Simulations

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This work leverages the high computational power of the supercomputer FUGAKU in combination with the Building-Cube Method (BCM) to carry out large-eddy simulations (LES) that assess the likelihood of ignite in a target aviation engine combustor. The inquiry focuses on examining the distribution of the equivalence ratio, which can serve as an indicator of ignition occurrences. The utilization of BCM, particularly the ”CUBE” framework developed by the Riken Center for Computational Science (RCCS), is an essential feature of this study since it enables rapid and realistic simulation of intricate engine designs.

This work is currently progressing towards comprehensive combustion modeling. However, the current emphasis is on investigating the dynamics of spray particles using an Euler-Lagrangian approach, with n-Dodecane being used as the fuel. This approach provides initial observations regarding the feasibility of reaching ignition.

In addition, the compressible immersed boundary approach (IBM) is employed to efficiently handle the complex geometry of aviation engines. The presentation will also address prior research that has played an essential

role in enhancing the use of large-scale spray combustion LES, accurately capturing the complex features that define aviation engine combustors.

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Performance Evaluation of Aero Engine Combustor by LES Integrating Turbulent Atomization Model

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Performance requirements for jet engines are becoming increasingly severe, requiring the use of numerical simulations for rapid and efficient development. Increasing the scale of simulation and improving accuracy are required for development applications. In this study, integration of the fuel atomization process into combustion LES was focused to further improve the accuracy of performance prediction. Liquid atomization processes are elementary processes that have a significant impact on combustor performance, but the complexity of the phenomena makes it difficult to integrate them into turbulent combustion simulations. To integrate turbulent atomization into turbulent combustion calculations, the liquid behavior was calculated using Euler-Euler method and the droplets after atomization were calculated as Lagrangian particles. The process of atomization from the Eulerian phase liquid is described by a LES subgrid type turbulent atomization model. Simulations were performed for kerosene combustion in a three-sector high-pressure combustor to evaluate the impact of the model. Simulation results confirm that the integration of the turbulence atomization model has a significant effect on the combustion behavior in the vicinity of the injector. This is because the turbulence atomization model affects the fuel/air mixing behavior at the flame tip, which also affects emission prediction.

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Numerical investigation of oxygen-hydrogen combustion with steam dilution for a zero-emission power generation system

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The oxygen-hydrogen combustion turbine cycle generates electricity by burning oxygen and hydrogen in a stoichiometric ratio with steam dilution. Therefore, this cycle is a zero-emission and carbon-free power generation system that does not produce nitrogen oxides (NOx) or carbon dioxide (CO2). In this study, large eddy simulation (LES) is performed for the entire flow field of the combustor in this cycle, including the cooling flow path, and the validity of the LES is investigated by comparing with the experiments. The results show that the present LES is capable of capturing the general behavior of the combustion-steam dilution-cooling flow fields in the combustor.

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Numerical simulation of boundary layer flashback of hydrogen-air premixed flame using an LES/NA-FGM-PD approach

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Prevention of flashback is one of the key issues for the Dry Low NOx (DLN) hydrogen-fired gas turbine combustor. In order to accelerate the combustor development, high-precision, and low-cost numerical simulation technology is required. Reproducing the boundary layer flashback of the hydrogen flame using computational fluid dynamics (CFD) is challenging because it requires resolving the turbulent boundary layer while considering the heat loss to the wall and the preferential diffusion effect. In this study, a large eddy simulation (LES) employing a non-adiabatic flamelet-generated manifolds approach considering the effects of heat loss and the preferential diffusion, referred to as an NA-FGM-PD method, is applied to simulate hydrogen-air premixed flame propagating in a rectangular channel. Then, the validity of the NA-FGM-PD approach to predict boundary layer flashback is examined by comparing it with the experimental data. The results show that an NA-FGM-PD approach captures the flashback limit variation and flame behavior observed in the experiments, in which flashback occurred when increasing equivalence ratio or decreasing air flow velocity. This suggests that the NA-FGM-PD approach will be an effective tool in the development of DLN hydrogen-fired gas turbine combustors.

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Super-simulation of Coal Gasification Facility on Fugaku

Shinobu Yoshimura[1], Hiroaki Watanabe[2], Ryoichi Kurose[3], Tomonori Yamada[1], Shigeki Kaneko[1]

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In our work, we target one of innovative clean energy systems, i.e. carbon-free coal gasification plant. The coal gasification is one of the key technologies to drastically reduce CO2 emission from coal fired power generation. Coal is crushed into fine particulate matter and then partially burned into gas in a high-pressure and elevated-temperature environment. We perform a high-fidelity two-way coupled simulation of combustion turbulent flow and thermal conduction and cooling in a reactor vessel of a laboratory-scale coal gasification facility. We first explain our developed multiphysics and multiscale simulations on the Supercomputer Fugaku, which we call Super-simulation in short. Here a unique parallel coupler, REVOCAP_Coupler, is used to integrate highly parallelized independent solvers such as a FVM-based combustion LES flow solver, FFR-Comb, and a FEM-based thermal conduction and cooling solver, ADVENTURE_Thermal. The simulation results are quantitatively compared with experimental results obtained from the laboratory-scale experimental facility. We succeeded in quantitatively reproducing the experimental phenomena in the facility with regard to temperature distribution as well as generated chemical components. The developed simulations will be powerful tools to improve the design and operation of actual coal gasification plants.

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Multi-objective optimization of operating conditions and reactor configuration of gasifier for solid fuels using FUGAKU

Kenji Tanno[1], Satoshi Umemoto[1], Hiroaki Watanabe[2], Ryoichi Kurose[1]

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Among recycling technologies for plastics and other chemical products, gasification is one of the most promising recycling technologies because it can treat wastes that are difficult to recycle as materials and has very high efficiency because it is processed in a reactor at high temperature and pressure. However, suitable operating conditions and gasifier configuration vary depending on the properties of the feedstock. In this study, multi-objective optimization calculations based on the genetic algorithm were performed to investigate the optimal operating conditions and the gasifier configuration. CFD calculations were performed using Euler-Euler calculations with FrontFlow/red, and the multi-objective optimization algorithm was NSGA-II. Burner blowout velocity, oxygen concentration, steam concentration, and gasifier configuration were set as design variables, and the objective functions were maximize gas heating value, maximize H2/CO ratio, and minimize char volume. The results showed that Pareto fronts were observed for each gasifier geometry, indicating that multi-objective optimization calculations may be utilized for gasification reactor design.

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MS17 Machine learning techniques for reacting flow simulation and analysis

Organizers: Abdulla Ghani[1], Anh Khoa Doan[2], Hiroshi Gotoda[3]

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MS17-1 Machine learning techniques for reacting flow simulation and analysis (1)

Chair: Anh Khoa Doan
Co-Chair: Hiroshi Gotoda
Friday, May 10; 13:00 - 15:00; Room L

Data-driven identification of precursors of extreme events in reacting flows

Mihnea Khoa Floris[1], Tadikonda Shiva Sai Sai[2], Dibyajyoti Nayak[2], Ivan Langella[1], Konduri Aditya[2], **Nguyen Anh Khoa Doan**[1]

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Many combustion systems can exhibit extreme events which are events where the combustor exhibits large excursions away from its design point. Examples of such events are flame blow-out or flashback in hydrogen combustors. The prediction of such events is very challenging due to the complex chaotic and multiscale effects at the origin of these events and the limited observations we have of those.

In this work, we develop machine learning techniques to identify precursors of extreme events, and specifically we tackle the problem of flashback prediction in a lean hydrogen reheat combustor which exhibits intermittent flashback. We first use a co-kurtosis based approach to identify the features of the thermochemical and flow state which are the most relevant for the onset of flashback. This allows for an efficient low-dimensional representation. From this reduced representation, a modularity-based clustering algorithm is employed to segregate between clusters which contain normal and extreme (flashbacking) states, and the cluster located in-between these states, which are the precursor states of flashback.

We show that our approach is able to identify precursors of flashback that provide a prediction time relatively large compared to the duration over which the combustor is stable between two flashback events. The performance of our method when using shorter time series or other sets of features (such as those coming from measurable quantities) is also investigated.

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Synchronized state and formation mechanism of spray combustion oscillations in a backstepped combustor

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We examine the synchronized state and formation mechanism of spray combustion oscillations in a backstepped combustor from the perspective of symbolic dynamics and machine learning. We use the symbolic recurrence quantification analysis [Mori et al., Proc. Combust. Inst., vol. 39, p. 4671, 2023; Mori et al., Phys. Rev. Appl., vol. 19, 034097, 2023] and the causality analysis based on a random forest [Leng et al., Chaos, vol. 29, 093130, 2019] to the numerical results obtained by a large-eddy simulation [Kitano et al., Combust. Flame, vol. 170, p. 63, 2016; Pillai et al., Combust. Flame, vol. 220, p. 337, 2020]. A phase-synchronized state (desynchronized state) between the acoustic pressure and heat release rate fluctuations exhibits in the upstream region (downstream region) of the combustor. This is clearly identified in the recurrence rate on the symbolic recurrence plots. The causal analysis based on a random forest reasonably shows that the large-scale organized vortex motion significantly affects the mutual coupling between the acoustic pressure and heat release rate fluctuations with pseudo-periodic dynamics.

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Probabilistic Machine Learning for Data-Based Flame Dynamics Modeling

Axel Zimmermann, Alexander J. Eder, Camilo F. Silva, Wolfgang Polifke
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Accurately modeling flame dynamics is crucial for predicting thermoacoustic instabilities. While neural networks have demonstrated their effectiveness in reproducing the nonlinear dynamics of laminar premixed flames, their applicability to turbulent flames has yet to be demonstrated. The challenges in this application are manifold: Firstly, the sparsity of data, resulting from the high computational demand of reacting flow simulations; secondly, the presence of combustion noise resulting in noisy data; and thirdly, the 'black box' nature of these models raises questions about their reliability for industrial use.

In this study, we seek to address the aforementioned issues using Bayesian neural networks (BNNs). BNNs promise a significant advantage in this context due to their inherent capability to quantify uncertainty. Uncertainty estimation can provide insights into data requirements across various flame dynamics regimes, thus potentially reducing the overall required data. Moreover, with BNNs, combustion noise can be naturally modeled by choosing an appropriate likelihood function.

We first present the capabilities of the Bayesian approach on a laminar premixed flame. We train the network on broadband-forcing data and evaluate whether the predicted flame-describing function and the associated confidence intervals can be trusted. Subsequently, we show first results for turbulent flames.

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Data assimilation for reacting flows: Deep learning PDE models to augment turbulent combustion simulations

Priyesh Rajesh Kakka, Jonathan F MacArt
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The traditional Boussinesq and gradient-diffusion hypotheses in turbulence modeling struggle to accurately represent turbulent fluxes in premixed flames, mainly due to counter-gradient transport. Current methods to include heat-release effects in turbulence closures often rely on linear combinations of limit case models, indicating a need for a more adaptable, comprehensive approach for diverse turbulent combustion regimes. In response, we propose to augment traditional turbulence models with deep neural networks in a data assimilation framework. These networks are trained to improve low-fidelity partial differential equation (PDE) models using high-fidelity data by employing a PDE-constrained, adjoint-based optimization algorithm. This approach has proven to be effective for training turbulence models in both nonreacting large-eddy simulation (LES) and Reynolds-averaged Navier–Stokes (RANS) frameworks. A crucial element of this strategy is PyFlowCL, a high-performance solver for compressible turbulent reacting flows. It solves both the forward and adjoint PDEs, needed for model training, by leveraging automatic differentiation capabilities. We introduce a neural-network-aided RANS closure model and demonstrate its capability to predict the evolution of turbulent jet flames across a range of Damköhler numbers. The model's generalizability is further tested for out-of-sample cases, marking a significant enhancement in RANS model closures for turbulent combustion prediction.

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A Probabilistic Framework for Data Assimilation of Reacting Dynamical Systems using a Gaussian Process Regression-based Reduced-Order Model and Sparse Measurements

Alberto Procacci, Salvatore Iavarone, Laura Donato, Axel Coussement, Alessandro Parente
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The objective of this work is to develop a mathematical framework to assimilate sparse noisy measurements of a dynamical system with the prediction coming from a Gaussian Process regression-based reduced-order model, in a fully Bayesian fashion. The reduced-order model of the dynamical system is built by coupling dimensionality reduction, obtained using the proper orthogonal decomposition, and non-linear regression via Gaussian Process regression. The Gaussian Process regression is a Bayesian regression framework in which the prediction is modeled as a sample from a multivariate Gaussian distribution. This characteristic can be leveraged to represent the dynamical system as a stochastic model, by employing the mean and uncertainty of the predictive distributions as parameters of the model.

The sparse measurements are also modeled as a stochastic process represented by a multivariate Gaussian distribution. This let us assimilate the measured samples and the reduced-order model by conditioning its predictive distribution with the sparse measurements.

This framework is tested on a pulsating laminar non-premixed methane flame, in a nitrogen-diluted coflow. The results are compared with established methods for data assimilation such as the Ensembled Kalman Filter.

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Turbulence Fine-scale Reconstruction Using Learning Techniques

Andreas H Rauch, Anthony Carreon, Venkat Raman
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Turbulent flows are critical to engineering combustion applications, but numerical simulations of practical engineering devices cannot afford to resolve all turbulence and flame features throughout the domain. This motivates multiscale modeling approaches using adaptive mesh refinement (AMR). AMR enables the efficient simulation of a vast range of length and time scales through targeted refinement of local features. However, generating finer meshes using AMR alone cannot restore high wavenumber turbulence features at the interface between mesh levels. This requires super-resolution turbulence to provide high-fidelity inflow conditions to fully resolved regions. This work explores novel learning techniques to generate sub-grid scale turbulence for super-resolution boundary conditions. Shock-turbulence interaction simulations are performed at coarse and fine resolutions to generate matching training data pairs. Then, learning techniques, including a U-net model, are trained to generate sub-grid scale turbulence from an input coarse turbulent field, restoring fine-scale turbulent kinetic energy in the post-shock region, where the turbulent scales drastically reduce. This offers a computationally efficient approach for high-fidelity simulations of shock-laden reacting flows, including detonations and supersonic combustion.

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MS17-2 Machine learning techniques for reacting flow simulation and analysis (2)

Chair: Anh Khoa Doan
Co-Chair: Abdulla Ghani
Friday, May 10; 15:20 - 17:20; Room L

A Dynamic Data-Driven Mixed Model for the Subgrid-Scale Stress Tensor and Scalar Fluxes in Large-Eddy Simulation of Turbulent Lean Hydrogen Flames

Ludovico Nista[1], Fabian Fröde[2], Temistocle Grenga[3], Jonathan F. MacArt[4], Antonio Attili[5], Heinz Pitsch[2]
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Direct numerical simulations (DNS) have shown that turbulent lean hydrogen/air flames are prone to thermodiffusive instabilities, resulting in a highly wrinkled flame front and a substantial increase in flame speed. However, DNS is computationally prohibitive for engineering applications, necessitating reduced-order approaches, such as large-eddy simulation (LES). Conventional turbulent combustion LES models, though, face challenges in accurately simulating turbulent lean hydrogen flames, leading to a considerable discrepancy between LES and DNS. Ongoing modeling efforts have addressed many of the unclosed LES terms; however, models for the subgrid-scale (SGS) stress tensor and scalar fluxes still have severe shortcomings in regimes relevant to hydrogen combustion, where instabilities manifest across different scales, starting from small and growing to larger scales. Therefore, improving the modeling of these fluxes is crucial, and considering the super-resolution (SR) approach becomes fundamental to accurately reconstruct SGS fluctuations.

We propose a dynamic data-driven mixed model that combines an SR, machine-learning-based, scale-similarity model, which explicitly reconstructs SGS terms, and an eddy-viscosity type model. A priori tests for lean premixed turbulent hydrogen slot-jet flame show a high correlation of the instantaneous SGS stress and scalar fluxes with the corresponding DNS data. A posteriori LES simulations will be presented to assess the ability of the data-driven mixed model to represent the thermodiffusive instabilities and flame-turbulence interactions.

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Large-Eddy Simulation of flameless combustion with neural-network driven chemistry

Luc Vervisch[1], Huu-Tri Nguyen[2], Camille Barnaud[3], Danh Nguyen[4], Pascale Domingo[5]
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Large eddy simulation of a flameless combustion furnace is discussed with a comparison against experimental measurements of the mean thermochemical quantities. The focus is on introducing flow simulations of complex chemistry through the training of neural networks, to simulate the oxidation of a gaseous fuel representative of recycled gases available in the steel industry. A canonical problem, based on a non-adiabatic stochastic micro-mixing model and combined with a detailed chemistry description, is set up to train the neural networks before the flow simulation. For these networks to be predictive, the thermochemical composition space is automatically decomposed into sub-domains from a partitioning algorithm.

A neural network is trained in every sub-domain to return the increments in time of the most influential thermo-chemical quantities, from the knowledge of temperature and species mass fractions solved with the flow. Implemented in an open-source low-Mach number fluid mechanics code, the neural networks complex chemistry is shown to be very efficient in CPU time, with an overhead of only 60% compared to the non-reactive multi-species simulation of the furnace.

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A comprehensive study on the accuracy and generalization of deep learning-generated chemical ODE integrators

Ruixin Yang, Han Li, Zhi X Chen
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The application of deep neural networks (DNNs) shows significant promise as a viable alternative to directly integrating chemical source terms in combustion simulations. However, challenges persist in ensuring high precision and generalization across various fuels and flow conditions. In this study, we propose and validate a consistent DNN approach for integrating chemistry across a range of fuels and premixed flame configurations. This approach involves generating a thermochemical base state from a set of low-dimensional laminar flames, followed by an effective perturbation strategy to enhance coverage of the composition space for improved generalization. A constraint criterion based on heat release rate is then applied to eliminate nonphysical perturbed states, thereby enhancing overall accuracy. Without specific tuning, three DNNs are consistently trained for three representative fuels: hydrogen, ethylene, and Jet-A. Comprehensive validations are conducted using 1-D laminar flames and two typical turbulent premixed flames. The DNN model predictions for various physical characteristics, such as laminar and turbulent flame speeds, dynamic flame structures influenced by turbulence-chemistry interactions, and conditional scalar profiles, exhibit good agreement with results obtained from direct integration. This underscores the exceptional accuracy and generalization ability of the proposed DNN approach. Furthermore, when the DNN is employed in simulations, a significant acceleration in chemistry integration is achieved, with approximately a 50-fold increase for the ethylene/air flame and a 90-fold increase for the Jet-A/air flame.

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A combined PCA-CSP solver for dimensionality and stiffness reduction in reacting flow simulations

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In reacting flow simulations, reduced-order models (ROM) play a crucial role in enhancing our understanding of the physical processes and accelerating simulations. Data-driven Principal Component Analysis (PCA) for dimensionality reduction and the physics-based Computational Singular Perturbation (CSP) for temporal stiffness reduction have demonstrated their effective roles in accelerated computing without losing fidelity.

The present study proposes a new algorithm, that combines the benefits of both methods by a double mapping operation from the state-space to time-decoupled and lower-dimensional PCA-CSP latent variables. In this approach, the complex reactive system is first mapped onto the orthogonal space by the PCA projection, followed by the dynamical time-scale decomposition of CSP operated on the PC-score variables, such that the time integration is performed on the active modes using the G-scheme algorithm. The PCA-CSP methodology also introduces the concept of latent Jacobian, representing the Jacobian matrix in the latent space of PCA variables.

The approach is validated on an ignition test case of a homogeneous ammonia/air mixture with detailed chemistry. Significant computational savings are achieved through the eigenvalue decomposition of the much smaller latent Jacobian matrix of the PC scores, without loss of accuracy. The results suggest a potential for the PCA-CSP algorithm to achieve substantial acceleration of high-fidelity reacting flow simulations involving large number of variables with a wide spectrum of time scales.

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Physics-Informed Neural Networks for Turbulent Combustion: Extracting Closure from Multiscalar Measurements

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We develop a physics-informed neural network (PINN) to evaluate closure terms for turbulence and chemical source terms from temperature, major species, and velocity point measurements. The goal is to develop closure for the transport of momentum and the thermo-chemical state. We adopt a deep operator network (DeepONet)

to accommodate two sub-networks related to two inputs: the spatial coordinates and flame inlet parameters, including inlet velocities and recess lengths of the fuel inlet. The PINNs are trained on several Sydney Flames and validated on an additional flame. A relatively shallow network attached to PINNs is used to relate the unconditional means of the species to their source terms in their transport equations. Additional observations of the PINNs are evaluated for the species' reaction rates. The terms are evaluated by integrating the species' reaction rates conditioned on principal components (from principal component analysis implemented on experimental data) and the principal components' joint PDFs from the experimental data. The measured species' reaction rate conditional means are evaluated using OD simulations to recover non-measured species and evaluate reaction rates. The results show that the species, the mixture fraction, and the axial and radial velocity components can adequately be represented with PINNs compared to experimental statistics. Moreover, PINNs can reconstruct closure terms associated with turbulence and scalars' transport, including the species' chemical source terms.

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Sparse data and reactive flow physics-informed neural networks

Abdulla Ghani
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In this talk, I will present a new method to reconstruct reactive flow fields based on sparse data. To do so, we developed neural networks that incorporate governing equations for reactive flow fields, called reactive flow physics-informed neural networks (RF-PINNs). The goal is to perform flow field reconstruction using a minimal amount of data, e.g. a handful of velocity profiles obtained from PIV measurements. I will demonstrate the effectiveness of our method on multiple cases including laminar and turbulent flames, and discuss future work in this field.

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MS18 Data-driven tools for HPC simulations of e-fuels combustion

Organizers: Federica Ferraro[1], Alessandro Stagni[2]

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MS18 Data-driven tools for HPC simulations of e-fuels combustion

Chair: Federica Ferraro
Co-Chair: Alessandro Stagni
Friday, May 10; 09:50 - 11:50; Room H

A workflow for the semidetailed modeling of complex e-fuels: application to oxymethylene ethers

Alessandro Stagni[1], Timoteo Dinelli[1], Alessandro Pegurri[1], Andrea Bertolino[2], Alessandro Parente[2], Marco Mehl[1], Tiziano Faravelli[1]

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When the chemical complexity of e-fuels grows to a higher level, as is the case of oxymethylene ethers (OMEs), the resulting kinetic mechanisms might have a limited applicability due to their size. In this case, simplification techniques need to be implemented for their integration into HPC simulations. In this work, we show that the kinetic modeling of longer-chain fuels can be simplified to a great extent by building up a single workflow, based on i) the definition of a smaller, archetypal species (dimethoxymethane – or OME1); ii) the coupling between lumping techniques and analogy and rate rules, based on the archetypal species, to develop the reaction submodules of each OME; iii) a data driven optimization, based on reaction classes, retaining the consistency previously defined among the different modules.

Such a workflow proved able to finalize a semidetailed model, with accuracy features competitive with the literature mechanisms, as shown by the large-scale validation performed for each of the components of the OME family. At a second stage, this can be effectively coupled with skeletal reduction methodologies, to bring the size of the mechanism to acceptable levels for HPC applications.

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Leveraging data assimilation techniques to integrate experimental and synthetic measurements in the kinetic mechanisms of e-fuels

Timoteo Dinelli[1], Tiziano Faravelli[2], Alessandro Stagni[2], Matthias Ihme[1]

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The current development of kinetic mechanisms relies heavily on the data-driven optimization of kinetic rates, previously evaluated by direct measurements and quantum chemical calculations. Different methods have been developed to integrate information from experimental measurements into kinetic models, including the solution mapping method by Frenklach or the Method of Uncertainty Minimization using Polynomial Chaos Expansions by Sheen and Wang. Recently, the Bayesian approach has attracted significant attention in the chemical kinetics community, as it provides a probabilistic approach to quantify uncertainties from both prior knowledge and experimental data. In this context, data assimilation (DA) methods offer opportunities to integrate experimental and synthetic measurements into numerical simulations. Among the various DA techniques, the Ensemble Kalman Filter (EnKF) is selected for this research due to its ability to include quantities not contained in the solution vector, and its robust evaluation of the error covariance: it is a statistical method, applicable to large-scale inverse problems like the one faced in this research. To this end, we have explored the possible applications of EnKF to optimize rate parameters of kinetic mechanism for promising e-fuels candidates.

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Enhancing computational efficiency of laminar flames simulations through time-dependent bases

Eva Muñoz[1], Hessam Babaee[2], Alessandro Parente[1]
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Combustion is inherently complex, as it involves multiple scales and intricate physical processes, resulting in computationally expensive simulations in terms of both memory and CPU time. To address this challenge, reduced-order models play a crucial role in enhancing our understanding of the process and accelerating simulations.

This research focuses on reduced-order modeling using the time-dependent bases (TDBs) approach [1]. TDB solves species transport equations for basis vectors in a low-dimensional manifold. The method is data-free and designed to ensure that the projection operator adjusts and rotates to align with the instantaneous flow characteristics, making it potentially suitable for unsteady problems.

The objective of this study is to investigate the method potential for a range of fuels and operating conditions, identifying strategies to maximize the reduction potential of the approach. To this purpose, TDB approach is implemented in laminarSMOKE [2], an OpenFOAM-based software designed to solve laminar flames with detailed chemistry. The analysis covers CFD simulations of steady and transient laminar axisymmetric coflow diffusion flames burning mixtures of burning mixtures of H2, CH4, or n-heptane with N2 in air [3, 4].

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Evaluation of Neural Network Performance for Chemistry Closure through Domain Decomposition

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Artificial Neural Networks (ANN) are emerging as a data-driven alternative for the chemistry closure in CFD of reactive flows for their capabilities of learning the correlation between transported control variables and the full thermochemical state, including also the relevant chemical source terms.

However, ANNs are not directly trainable to a sufficient relative tolerance when the output quantities span multiple orders of magnitude, which is the case for chemical source terms.

To overcome this issue, previous works applied multiple networks, each responsible for a subset of the full chemistry manifold of the training data. It was observed that, with an increase in the number of subdomains, simpler networks are able to predict their respective subdomain with higher accuracy compared to a single network.

In this work, an ensemble neural network (eNN) model for predicting the species chemical source terms in reacting flows is presented. Specifically, the decomposition method, the accuracy of the resulting eNN, and the limitation of the approach are explored in a parameter study. The proposed closure is applied to test cases of increasing complexity for hydrogen-air mixture, including autoignition problems and laminar premixed flames that develop thermo-diffusive instabilities.

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Analysis of flamelet-based manifolds for turbulent H2-flames subject to thermo-diffusive instabilities

Hannes Böttler[1], Driss Kaddar[1], Jeremy Karpowski[1], Federica Ferraro[2], **Arne Scholtissek**[1], Hendrik Nicolai[1], Christian Hasse[1]
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While flamelet-based modeling techniques have been successfully applied in many scale-resolving simulations of turbulent hydrocarbon flames, transferring the approach to (lean) turbulent hydrogen flames still represents a challenge. One of the reasons is the fine-scale wrinkling of the flame front due to both, intrinsic thermo-diffusive instabilities and turbulence, which leads to an increase in the flame surface area and consequently the flame's

burning rate. In an earlier work, we have demonstrated the application of flamelet-based models to laminar thermo-diffusively unstable hydrogen flames, which has shown that including curvature effects in the generation of the manifold leads to improved model predictions. In the present work, we analyze this modeling technique for a turbulent hydrogen flame. A DNS of a turbulent lean premixed hydrogen-air slot flame with finite-rate chemistry is carried out first. The flame's thermochemical state is examined using a composition space model, separately considering effects from strain and curvature. An a-priori analysis confirms that the previously developed tabulated manifolds fall short of capturing all the turbulent flame phenomena. An extended manifold, spanned by control variables for mixing, reaction progress, strain, and curvature, is shown to improve the results significantly. With this, the present work provides novel insights into the required manifold complexity for capturing the physics of turbulent lean hydrogen flames.

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A universal LES subfilter model based on AI super-resolution and application to hydrogen flames

Mathis Bode[1], Bogdan Danciu[2], Christos Frouzakis[2]
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The green energy transition requires the adaptation and optimization of many combustion applications. In particular, the switch to hydrogen as a carbon-free fuel is a key task here. This is not possible without the combination of highly accurate direct numerical simulations (DNS) to understand physical phenomena in detail and reduced models, especially large-eddy simulation (LES), to address real-world applications. Physics-informed enhanced super-resolution generative adversarial networks (PIESRGAN) are a promising approach to systematically derive general LES subfilter models from DNS data. The general idea is to train an AI network with different datasets in such a way that it is able to "reconstruct" DNS-like resolution from filtered data. This allows super-resolution of data in an a priori sense and the accurate prediction of the temporal evolution in an a posterior sense by closing the LES equations using the AI super-resolution subfilter model. This work presents a universal derivative model and its application to hydrogen flames. Besides the prediction of complex chemistry, a focus is on the simultaneous correct modeling of turbulent flow in complex geometries. The universal subfilter model results in an extremely good prediction accuracy and can significantly speed up complex simulations.

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MS19 Tabulation Methods for Homogeneous and Heterogeneous Reacting Flow: Machine Learning and Other Approaches

Organizers: Stelios Rigopoulos[1], Francesca Di Mare[2], Fabian Sewerin[3]

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MS19 Tabulation Methods for Homogeneous and Heterogeneous Reacting Flow: Machine Learning and Other Approaches

Chair: Stelios Rigopoulos
Co-Chair: Fabian Sewerin
Friday, May 10; 09:50 - 12:10; Room L

Machine Learning Tabulation of Chemical Kinetics for Turbulent Combustion Simulations

Stelios Rigopoulos, Thomas Readshaw, Tianjie Ding, William Philip Jones
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The computation of turbulent flames with methods that involve direct coupling of chemistry and flow is a very computationally demanding task, especially for large and complex mechanisms that are often required to simulate combustion of commercial fuels, soot formation and new sustainable fuels. We show the progress of a methodology, the hybrid flamelet/random data and multiple multilayer perceptrons (HFRD-MMLP) method, developed within our research group for a number of years, which employs machine learning to replace the real-time computation of thermochemistry. As such, it is applicable to methods such as Direct Numerical Simulation (DNS), Probability Density Function (PDF) methods, unsteady flamelet, Conditional Moment Closure (CMC), Multiple Mapping Closure (MMC), Linear Eddy Model (LEM), Thickened Flame Model, the Partially Stirred Reactor (PaSR) method (as in OpenFOAM) and the computation of laminar flames. The fundamentals of the method are explained and a number of case studies are shown for different types of turbulent flames, fuels and reaction mechanisms. The large eddy simulation (LES) – PDF approach is employed, together with the stochastic field method for numerical solution. It is shown that accurate results can be achieved for both major and minor species, with a 10-50 times acceleration of the chemical reaction step.

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Criteria to switch from tabulation to neural networks in computational combustion

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Motivated by the need to reduce computational costs, look-up tables are widely used in numerical simulations of laminar and turbulent flames, for the thermodynamics of the mixture, for detailed chemistry, and for turbulent combustion closures. At the same time, there have been many studies where artificial neural networks have been trained to replace the classic tabulation approach, and their performance against tabulation is typically evaluated afterward. The computational efficiency is an important ingredient, and criteria are needed to decide whether or not it is worthwhile in the first place to employ neural networks at all, and if so what the potential bounds on the computational time and memory gains (if any) over tabulation are. Analytical expressions will be presented for the computational cost of tabulation and of neural networks including the effect of network structure. The scaling laws are validated using both model test-data but also data based on a canonical problem which involves inferring laminar flame speeds of methane/hydrogen mixtures at off-training conditions. The proposed scaling laws lead naturally to a framework for effective decision-making between adopting look-up tables or neural networks.

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Classification of thermochemical states in turbulent premixed combustion using autoencoder neural networks

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Low-dimensional modeling (LDM) of the thermochemical variables, such as Flamelet Prolongation of Intrinsic low-dimensional manifolds (FPI) and Flamelet Generated Manifold (FGM), are very useful for combustion simulations, especially when the chemical mechanism is complex. A crucial ingredient for LDM is the choice of low-dimensional representations (i.e., controlling variables), conventionally determined by prior knowledge or principal component analysis (PCA). Controlling variables determined by prior knowledge are easy to understand and straightforward to implement in LDM. E.g., a progress variable is used to determine the progress of the flame. However, when the thermochemical states – for instance when considering detailed transport models – become complex, additional controlling variables – out of prior knowledge – are needed to obtain an accurate representation. PCA is able to identify low-dimensional representations without any prior knowledge. Since PCA is in principle a linear regression, it is well suited for linear problems, but shows limitations for non-linear processes. In contrast to PCA, an autoencoder neural network (AENN) offers a suitable representation for non-linear problems as well. In this work, an AENN has been used to obtain the low-dimensional representations of the intricate thermochemical states found during turbulent premixed combustion. Up to now it is difficult to interpret the physical meaning of the latent space in the data-driven reduced dimensions. Therefore, a direct application of autoencoder as LDM – to replace FPI and FGM – is not really feasible. On the other hand, the present study takes the benefit of an AENN to classify the thermochemical states based on an automatic sensitivity analysis (automatic differentiation) of the thermochemical variables on the data-driven reduced dimensions. In this way, the controlling thermochemical variables can be identified at every local position and grouped to indicate different combustion process, e.g., ignition, local extinction, flame propagation. Validation of this technique is performed for NH3/H2/air premixed flames, which are of increasing interest for future carbon-free combustion.

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Harnessing a reduced order representation to solve the spatially inhomogeneous population balance equation

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Aerosols are frequently characterized in terms of a particle size distribution whose spatial and temporal evolution is governed by a population balance equation (PBE). Physically, the PBE synthesizes spatial particle transport due to advection and diffusion with localized particle formation, growth, breakup or coagulation. A particular challenge associated with the numerical solution of the PBE in a Eulerian framework is the economical parameterization of the particle size distribution in terms of a finite number of scalars, affording a size-discrete approximation. With the objective of minimizing the number of scalars, we present a novel reduced order representation of the particle size distribution that involves the notion of size-characteristics and is informed by training solutions of the PBE acquired in simplified reactors. The shape functions underlying the reduced order representation are identified using a proper orthogonal decomposition (POD) of the training dataset, while the scalars' evolution equations are obtained from a constrained Galerkin projection of the PBE. Considering the dispersion and growth of an aerosol in a laminar plane jet flow, we demonstrate that the PBE-POD solver requires about four times fewer scalars to achieve a given accuracy than adaptive grid methods. While the achievable accuracy is limited by the adequacy of the training dataset, the PBE-POD method delivers, by design, the best least-squares approximation of the exact solution in terms of the chosen shape functions.

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Modeling of Turbulent Reactive Flows Using a Self-Learning Reduced Order Model

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Many applications in turbulent combustion rely on some form of reduced order model. Flamelet-type models with pre-computed, tabulated chemistry are widely used and perform well. However, the creation of an appropriate and accurate table requires considerable knowledge and time. Data-driven models have shown a lot of promise in reducing this work. They are fast, simple to use, and can

provide high accuracy. But the result is often a black box. What is more, data-driven extrapolation to new, unknown data is not obvious. A feature required in most applications.

In this work, we implemented the RONAALP algorithm (Reduced Order Nonlinear Approximation with Active Learning Procedure) which combines off-line training with a self-learning approach to handle extrapolation events on-the-fly. The off-line training relies on a combination of nonlinear auto-encoders, community clustering, and radial basis function networks to develop an efficient and compact base model from limited training data. The active learning procedure expands the base model to consider extrapolation outside of the original training data. The algorithm was developed and validated for hypersonic flows in non-equilibrium. We transferred the methodology to turbulent reacting flows, training the model on 1D flamelet data, and using a direct numerical simulation (DNS) of two parallel turbulent premixed methane/air flames with flame-wall interaction as validation.

The base model performs as well as the original tabulation, without the effort of constructing the appropriate table. Due to the defined extrapolation procedure, active learning with either DNS data or additional flamelet data improves the predictions.

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Data driven modelling of sub-grid micro-mixing for PDF methods

Salvador Navarro-Martinez[1], Tin-Hang Un[2]

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Probability Density Function (PDF) methods have been proven successful in modelling combustion in a wide range of configurations. Using a sub-grid joint scalar PDF, the approach can close the filtered reaction source term exactly. Moreover, by including velocities into the joint PDF, the method yields a unified turbulence-chemistry interaction model. These methods are very general and have good synergies with chemistry tabulation methods. However, the sub-grid PDF transport equation is not fully closed and requires modelling. Most of the literature used the Simplified Langevin Model approach, which assume isotropy at the smallest scales and depends on filter width, sub-grid kinetic energy and a triad of RANS-calibrated constants. A more general model requires closure of the Langevin tensor, which includes the turbulent dissipation. This is a very complex parameter to model due to its intermittent nature, but crucial in modelling extreme events such as extinction and ignition. This work explores the use of small Deep Neural Networks (DNN) to represent a Generalised Langevin Model. A realisability constrain is imposed to link dissipation and sub-grid Reynold stress. The Reynolds stresses and velocity gradients are used as input data of the network. The DNN is trained with forced isotropic turbulence DNS at three different Reynolds numbers, with different filtering criteria. The new model shows good agreement with unseen DNS data and outperforms the SLM at several resolutions.

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Evaluation of Breakpoint Optimization Procedure for High dimensional Flamelet Tables

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High-dimensional flamelet tables improve the applicability of the flamelet based models, but increase in memory size of the table is important issue for massively parallel computing. In this study, breakpoint optimization procedure for high-dimensional flamelet tables has been developed, to optimize the balance between memory size and accuracy of the table. In order to improve an accuracy of the optimization, process of obtaining abundant solutions of counterflow diffusion flames is automated. Constrained nonlinear optimization algorithm is applied for process of finding optimal breakpoints of the table. Several conditions of the number of breakpoints in each control parameter of the table and objective functions in the optimization are evaluated. A priori analysis using the optimized flamelet table of flamelet progress variable approach which implemented in a compressible flow analysis solver is conducted for a H2/O2 flame. Finally, the same framework will be applied to the flamelet table of quasi-two-dimensional flamelet model.

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MS20 Modeling and Simulation of High-speed Compressible Reacting Flows

Organizer : Venkat Raman
University of Michigan

MS20 Modeling and Simulation of High-speed Compressible Reacting Flows

Chair: Venkat Raman
Thursday, May 9; 09:50 - 12:30; Room K

Stability and Dynamics of High-speed, Compressible, Premixed and Non-premixed Turbulent Reacting Flows

Alexei Poludnenko
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In a wide range of practical systems, from hypersonic scramjet engines to detonation-based combustors, turbulent reacting flows operate in rather extreme, high-speed, highly compressible regimes. In this talk, we discuss several phenomena characteristic of such regimes, which were discovered in recent years using direct numerical simulations. In particular, we show that premixed turbulent flames can develop pulsations with significant peak-to-peak amplitudes. Such unstable burning can result in the pressure build-up and the formation of shocks, ultimately even driving transition to a detonation, when the flame speed approaches or exceeds the speed of a Chapman-Jouguet deflagration. Recent results also show existence of a similar unstable burning regime in non-premixed flames. Such instability is intrinsic to a flame, and it can develop even in the absence of the surrounding combustor walls or obstacles. Furthermore, coupling of pressure and density gradients, as well as heat-release-driven dilatation across the flame can lead to the anisotropic generation of turbulence inside the flame volume and flame acceleration. In particular, we show that this process can result in turbulent flame propagation and substantial self-acceleration even in the absence of the upstream turbulence. We discuss the physical mechanisms behind these phenomena along with the implications of these results for subgrid-scale LES combustion models.

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Effect of Fuel Dispersion on Reaction Structure in Supersonic Flowpaths

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Efficient combustion is a major challenge in the development of hypersonic vehicles. Single transverse injectors face limitations in the mixing uniformity, thereby impacting the combustion efficiency. Multiport injection schemes lead to the formation of complicated shock structures formed by the interaction and reflection of the individual bow shocks generated due to the blockage of the jets. These curved shocks enhance the vorticity generation process, and their interaction with the jet fuel plumes downstream further strengthens the existing vortical structures, leading to enhanced mixing. These configurations, however, suffer from greater pressure losses and suppression of jet penetration due to the influence of opposing jets. This work aims to investigate the influence of different jet-to-crossflow momentum ratios on multiple sonic ethylene jets issued into a Mach 3 crossflow using an adaptive mesh refinement (AMR) based compressible flow solver with detailed chemistry. The analysis will focus on the influence of the momentum ratio and turbulence on the mixing, ignition characteristics, and reaction zone structure for the multiple injector configuration. AMR is employed to resolve the shocks, shear layers, and reaction front locations, preserving an overall fidelity comparable to direct numerical simulation while concurrently maintaining a computational cost akin to large eddy simulation.

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High-Order Discontinuous Galerkin Methods for Compressible, Chemically Reacting, Multicomponent Flows

Eric J Ching, **Ryan F Johnson**
US Naval Research Laboratory, United States

This talk presents a nonlinearly stable, high-order discontinuous Galerkin (DG) method for the chemically react-

ing, compressible Navier-Stokes equations. The following nonlinear-stability properties are mathematically guaranteed: boundedness of species mass fractions, positivity of density, positivity of pressure, and boundedness (from below) of specific thermodynamic entropy. Satisfaction of these properties allows for adequate suppression of numerical instabilities and discrete conservation of mass, total energy, and atomic elements over a wide range of meshes and polynomial orders. In addition, the methodology effectively maintains pressure equilibrium in smooth regions of the flow. Operator splitting is employed to handle stiff chemical reactions. The resulting formulation is compatible with curved elements of arbitrary shape, a variety of numerical flux functions, general quadrature rules with positive weights, and mixtures of thermally perfect gases. Several test cases involving reacting and non-reacting multicomponent flows are computed in a robust, conservative, and accurate manner, ranging from one-dimensional shock-tube and thermal-bubble-advection problems to multidimensional moving detonation waves, chemically reacting shock/mixing-layer interaction, and reacting jet in supersonic crossflow. This talk will conclude with discussions on DG's effectiveness, lessons learned in pursuing DG for propulsion simulations, and its potential role as a future design tool.

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LARGE EDDY SIMULATION (LES) OF HIGH SPEED COMPRESSIBLE REACTIVE FLOWS

Christer Fureby
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Large Eddy Simulation (LES) has rapidly evolved as a powerful computational method for high-speed compressible reactive flows, in-between Direct Numerical Simulation (DNS) and Reynolds Averaged Navier Stokes (RANS) in accuracy and cost. These flows are extremely challenging due to the combined complexities of turbulent compressible flow and combustion chemistry, putting additional requirements on the numerical schemes used. Here we will review the physical processes involved in high-speed compressible reactive flows and discuss the requirements for modeling each of these processes. Also to be commented on, is the interplay between the physics modeling and the need for low-dissipation schemes with ability to capture shocks and other flow discontinuities. Particular attention will be paid to phenomena not usually considered in LES of high-speed compressible reactive flows such as thermal radiation and thermal combustor-wall boundary conditions. Results from a small selection of experimentally investigated supersonic combustion cases will be presented, and the sensitivity to chemical reaction mechanisms, LES combustion models, thermal radiation modeling and thermal combustor-wall boundary conditions will be illustrated and discussed. Qualitative and quantitative comparison with experimental data will guide formulating a set of suggestions regarding how to make appropriate judgements when selecting the required physical model-ing details and set-ups.

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Chemical Kinetic Modeling for High-Speed Compressible Combusting Flows

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High-speed compressible combusting flows are characterized by a significantly broadened thermochemical state space. Accurate combustion chemistry modeling in these flows is challenging in two aspects. First, the frequent local extinction and ignition sensitize hierarchical chemistry to an extent that testing a combustion chemistry model against a small set of legacy combustion property data (e.g., laminar flame speed, shock tube ignition, counterflow extinction) is insufficient for validating its accuracy over the broader thermochemical state conditions which can be encountered in high-speed flows. Second, the broadened thermochemical state space also renders conventional model reduction strategy inadequate. To address these problems, we discuss our recent Foundational Fuel Chemistry Model 2 (FFCM-2) effort, focusing on optimization of a comprehensive H2, H2/CO, C1-4 reaction model through data assimilation followed by uncertainty quantification and minimization. In addition, we explore an approach that combines low-dimensional manifold identification with deep neural network training to obtain reduced models for computational fluid dynamics.

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Modelling strategies for Large Eddy Simulation of high-speed reacting flows

Salvador Navarro-Martinez
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Numerical simulation of high-speed reacting flows has many challenges. High-Reynolds number flows requires turbulence modelling. In scramjets mixing fuel and oxidiser is incomplete due to short residence times and finite rate effects are important with strong turbulence-chemistry interaction, with large non-linearities in the reaction

rates. Similarly, in rocket-type cryogenic injectors, non-ideal equations of state introduce complex relations between the thermodynamic properties. In LES, all these turbulence interactions require modelling and implementation in a solver. The simulations require resolving shocks, thin mixing layers and turbulent eddies simultaneously. To maintain stability, numerical schemes add artificial dissipation, but this process introduces erroneous mixing and dissipates turbulence. This numerical dissipation mask turbulence modelling and artificially coarsen unresolved scales and can, for example, accelerate the flame or cause blow-off. Sophisticated modelling approaches may be wasted if dissipative solvers are used. Numerical dissipation can act as an implicit sub-grid modelling (ILES); however, it can misrepresent behaviour close to walls or in unresolved regions. The main bottleneck is how to identify a-priori the behaviour of the combined numerical model-solver. This work explores modelling strategies on a scramjet configuration, including the effects of several numerical schemes, mesh resolution and combustion models: ILES, PaSR and PDF approaches.

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An analysis of non-premixed ethylene-air flame stabilization in a cavity flameholder with orthogonal fuel injection

Priyabrat Dash, Konduri Aditya
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Ramjet and scramjet engines are critical for the next generation of high-speed air travel. In scramjets, the flow is decelerated from a hypersonic freestream Mach number to a lower supersonic Mach number at the combustor entry. To stabilize flames within the combustor, cavity flameholders are employed. It is imperative to glean fundamental insights into such flame stabilization across operating conditions. To do so, we use high-fidelity simulations of cavity-stabilized non-premixed ethylene-air flames inside a model combustor resembling a jet-in-crossflow configuration at nominal flow conditions. The combustor geometry comprises a rectangular cross-section with a ramp-cavity, and two injectors (pilot and main) to introduce the fuel. The simulations are conducted using the open-source massively parallel code PeleC, incorporating a 22-species reduced order mechanism with 206 elementary reactions. We assess the sensitivity of flame anchoring toward perturbations caused by the pre-combustion shock train by mimicking its unsteadiness in the inlet conditions. The combustion characteristics and the role of the recirculation zone in assisting ignition at the flame anchoring point are studied. Additionally, we conduct a detailed investigation of the progress of individual reactions and the production/consumption of reacting species.

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Effect of a Turbulent Chemistry Interaction Model on Prediction of Scramjet Combustor Flows

Masatoshi Kodera, Masahiro Takahashi, Kan Kobayashi, Sadatake Tomioka
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Combustion tests for an ethylene fueled scramjet combustor with cavity flameholders used for a flight experiment have been conducted at Ramjet Engine Test Facility (RJTF) of JAXA under Mach 6 flight conditions using two types of airflows, clean air (M6S) and vitiated air (M6V). M6V is generated by H2/O2 combustion containing water vapor, while M6S is generated by a thermal storage heater. The RJTF results showed pressure rise due to combustion was lower at M6V in the cavity and downstream diverging combustor sections compared to M6S. On the other hand, RANS CFD assuming laminar combustion was not able to reproduce the difference between the two conditions obtained from the RJTF tests even if turbulent Schmidt number and turbulence model were changed. Therefore, we incorporated a partially stirred reactor (PaSR) model, which is one of the Turbulence Chemistry Interaction (TCI) models, into the CFD. Application of this model improved the agreement with the RJTF results in terms of the wall pressure distributions of the combustor. In this study, we will focus on the effect of the TCI model on the simulation of scramjet combustor flows and discuss the results in detail.

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Track01 Laminar flames

Track01-1 Laminar flames (1)

Chair: Jeroen Van Oijen
Wednesday, May 8; 10:40 - 12:20; Room M

Stabilization of flames in narrow channels by a highly conductive wall segment: effect of the Lewis number and application to hydrogen-air flames

Carmen Jimenez
CIEMAT, Spain

In this work, we study the effect of the Lewis number in the stabilization of premixed flames in narrow channels by a wall segment of finite length with high thermal conductivity and thermal capacity. The thermal conductivity of this wall segment is assumed to be so high that the temperature inside it is uniform. First, the auxiliary problem of flame stabilization at a given temperature of a highly conductive wall segment is considered and the total heat flux in this segment is calculated. It is shown that the heat flux becomes zero for certain values of the imposed temperature. These temperature values correspond then to solutions of the original problem, where the conductive wall segment is in contact only with the flame and is isolated from the external environment.

We show that for low Lewis number flames, this novel concept for flame stabilization only by thermal means provides stable operation for a wide range of values of the reactants flow rate, giving a large flexibility in terms of power output variation and exceeding the performance found in classical heat recirculating devices. We also show that multiple steady-state flame solutions may appear, which can complicate the operation of these devices.

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Flame stabilization by a highly conductive cylinder: multiple steady-state solutions and dynamics

Vadim N. Kurdyumov, Anne Dejoan, Carmen Jiménez
CIEMAT, Spain

This study examines stabilization of a premixed flame by a circular cylinder placed perpendicularly to the uniform flow of the reacting mixture. It is assumed that the cylinder has high thermal conductivity. Its temperature is not fixed, but it is determined by a thermal flame-cylinder balance. The numerical investigation is carried out on the basis of low Mach number Navier-Stokes equations coupled with the conservation equations for the energy and the fuel mass. Two models for transport coefficients are compared. The first model assumes they have constant values, and the second takes into account their change with temperature.

Numerical modeling shows that within the specific range of parameters of this study the system can have several steady-state solutions corresponding to different cylinder temperatures. Moreover, at least two solutions are shown to be stable, the two solutions corresponding to the hottest and coldest cylinder temperatures. The actual occurence of one or another regime depends on the initial conditions.

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Effect of the exhaust gases boundary condition on the stability and propagation regimes of a premixed flame in a slender chamber

David Rodríguez-Gutiérrez[1], Raquel Gómez-Miguel[1], Eduardo Fernández-Tarrazo[2], Mario Sánchez-Sanz[2]
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This work presents a numerical analysis of the propagation of laminar premixed flames in slender semi-open chambers. The study aims to evaluate the influence of the boundary conditions in the combustion process.

For this task, the combustion process is initiated with a local temperature raise close to the open end of the chamber. When activation temperature is reached, a

self-sustained combustion process begins, forming a flame that propagates along the chamber. Noise introduced into the system during ignition in the form of pressure waves interact and perturb the flame. The growth of these perturbations can induce thermos-acoustic oscillations in the flame and even modify the flame propagation regime.

All these phenomena has been studied using a constant pressure outlet boundary condition, an extensively used boundary condition for internal flows. However, given the strong non-linear nature of the reactive-flow, the thermo-acoustics and stability of the freely propagating flame problem, the use of this boundary condition can compromise the accuracy of the solutions obtained, as phenomena taking place at the chamber exit is not resolved: pressure wave reflections, flow entrainment or pulsating jets.

These overlooked phenomena can have a strong impact in the evolution combustion process itself. To evaluate this impact a domain surrounding the channel is added, accounting for the external atmosphere, being able to accurately resolve the exhaust low speed jet. A comparison with published constant pressure outlet results is carried out, providing an initial assessment of the impact the chamber exit phenomena has on the combustion process.

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Darrieus-Landau instability in a shear flow

Prabakaran Rajamanickam, **Joel Daou**
University of Manchester, United Kingdom

The Darrieus-Landau instability of premixed flames propagating in a narrow Hele-Shaw channel in the presence of a strong shear flow is investigated, incorporating also the Rayleigh-Taylor and diffusive-thermal instabilities. The shear flow also induces Taylor dispersion which results in anisotropic diffusion.

To understand how the anisotropy affects flame stability, two cases are considered, namely flame propagation in (1) the streamwise and (2) the spanwise directions. The analysis is based on a two-dimensional model derived by asymptotic methods and solved numerically, to characterise the influence of the flow Peclet number Pe, the Lewis number Le and the Rayleigh number Ra. Dispersion curves characterizing the perturbation growth rate are computed for selected values of Pe, Le and Ra.

Taylor dispersion is found to suppress the Darrieus-Landau instability and to weaken flame wrinkling when the flame propagates in the streamwise direction. In contrast, for spanwise propagation, the flame is stabilized in Le<1 mixtures, but destabilized when Le>1. For spanwise propagation, stagnation points and counter-rotating vortices are encountered in the flame near the unburnt gas side. It is shown that vorticity can be produced by a curved flame in a Hele-Shaw channel even without gravity, and that it remains confined to the flame.

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Diffusive-thermal instabilities of premixed flames in channel flows: 3D stability investigation and flow-induced anisotropic diffusion effects

Joel Daou, Prabakaran Rajamanickam, Aiden Kelly, Julien Landel
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The presentation comprises two studies related to the diffusional-thermal instabilities of premixed flames:

(1) an investigation of the influence of the direction of a shear flow relative to that of flame propagation in narrow channels and (2) a 3D analysis of the instabilities of flames propagating along the flow direction in channels of arbitrary width.

The first study compares analytically derived stability results with simulations involving the Lewis number Le, the Peclet number Pe, and the angle between the direction of propagation and the flow direction. Cellular instabilities expected when Le < 1 are now found to occur due to Taylor dispersion in Le >1 mixtures, provided the angle exceeds 75 degrees.

The second study examines flames in a Poiseuille flow. The instability is found to be a combination of the traditional diffusive-thermal instability and a recently identified transition from symmetric to asymmetric flames. Instability regions are identified in the Le-Pe plane. In narrow channels, it is found that flames are always symmetric with Taylor dispersion enhancing the cellular instability in Le < 1 mixtures and suppressing the oscillatory instability when Le >1. In large-scale channels, both instabilities persist with stronger propensity for asymmetry when the flow opposes flame propagation and Le<1.

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Track01-2 Laminar flames (2)

Chair: Ronan Vicquelin
Thursday, May 9; 09:50 - 12:30; Room M

DMD analysis on quasi-steady behaviors of sporadic flames in counterflow under low-speed low-Lewis-number conditions

Takaki Akiba, Akira Tsunoda, Youhi Morii, Hishashi Nakamura, Kaoru Maruta
Tohoku University, Japan

The quasi-steady ball-like flames in counterflow at low Lewis number was observed in microgravity experiments and named sporadic flame, and they were also confirmed in three-dimensional numerical simulation with diffusive thermal model at Lewis number lower than or equal to 0.5. The DMD (dynamic mode decomposition) analysis was applied for the temperature distribution of these sporadic flames in a quasi-steady state in order to understand their seemingly chaotic behaviors. The DMD analysis unveiled three predominant unique modes in the sporadic flames: (I) planar, (II) radial, and (III) circular modes. The decomposed modes showed two distinct spatial segments; the area forming sporadic flames near the counterflow axis and the area splitting and transporting flame pieces at outer part of the counterflow field. Furthermaore, fast Fourier transform (FFT) analysis was employed to examine the characteristic length scales of these decomposed modes, specifically the (II) radial and (III) circular structures. FFT analysis quantified identical characteristic length scales in both radial and angular directions, indicating a consistent scale across different spatial orientations within these distinct flame structures. This symmetry suggests underlying principles and essential symmetries governing these chaotic flame dynamics in counterflow fields.

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Measurement of Laminar Burning Velocity for pre-mixed fuel air mixtures at elevated temperatures and pressures

Subhashree Sampath
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Adding hydrogen to methane improves combustion efficiency, lowers carbon emissions, and supports a shift to cleaner and more sustainable energy practices. The present investigation reports numerical study using ANSYS CHEMKIN PRO software on laminar burning velocity variation of CH4+H2+air mixtures at elevated temperatures (300 K - 650 K) and pressures (1 - 5 bar). Hydrogen is blended with methane gas to reduce carbon emission into the atmosphere, to improve the flammability characteristics and subsequently combustion performance. The effect of mixture equivalence ratio (0.7 to 1.3) and H2 fraction (10% to 50% by volume) have been reported at elevated temperatures and pressures using chemical kinetic models like GRI Mech 3.0 and FFCM -1 and have been compared with existing literature data. The obtained results show that variation of equivalence ratio has a direct effect on the flame speed. It can be observed that as the dilution ratio of H2 increases there is an increase in flame speed due to the high diffusivity of hydrogen. This increase is due to faster formation of reaction radicals of H2, O and OH . When it comes to pressures, it can be noted that there is a decrease in the burning velocity value with an increase in pressure due to suppression in energy of the species in the reactants that slows down the flame propagation. Flame speed varies linearly with the temperature ratio due to increase in kinetic energy of molecules in the combustible mixture.

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Numerical investigation of effects of pressure and equivalence ratio on laminar hydrogen flame flashback behavior

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Kyoto University, Japan

These days, a hydrogen-fueled combustor is gathering attention as a key technology to achieve carbon neutrality. For the development of hydrogen-fueled combustors, predicting and preventing the occurrence of a flashback is one of the most challenging issues. However, the flashback behavior is dramatically different depending on the conditions, such as the equivalence ratio, the ambient pressure, and the unburnt gas temperature. Therefore, further research on flashback under various conditions is required for a thorough understanding of the fundamental properties of flashback behavior. In this study, the effects of equivalence ratio and ambient pressure on a hydrogen flame flashback and their interaction are investigated in detail. Two-dimensional numerical simulations of hydrogen-air premixed flame flashback in laminar channel flow are performed under various equivalence ratios and ambient pressures using a detailed reaction mechanism that includes 9 chemical species and 19 chemical reactions. The results show that the equivalence ratio and ambient pressure affect the flashback speed, critical condition of the flashback occurrence, and formation of the backflow regions.

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Flashback limits of H2 premixed laminar flames: a numerical investigation based on the "1+M" multi-component diffusion model

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Molecular diffusion is known to be a key process in combustion. The estimation of mass diffusion fluxes in multidimensional simulations including detailed chemistry is usually carried out using the mixture-averaged model. On the contrary, because of its high computational cost, the complete multicomponent formulation has been mainly used in 1D calculations only (especially when the number of chemical species is large) [1].

In this work, we explored a novel multicomponent diffusion model, referred to as "1+M" formulation [2], able to ensure accuracy levels similar to the complete formulation at the same cost of mixture-averaged. In particular, the numerical analyses were focused on the description of flashback occurring in laminar premixed flames fed with pure H2. More specifically, 3D numerical simulations were carried out on a multi-hole geometry that emulates perforated burners commonly found in domestic condensing burners. The simulations, including detailed kinetics and conjugate heat transfer with the burner plate, considered a range of equivalence ratios from 0.50 to 1 and various hole-to-hole distances for a more comprehensive analysis. The results confirmed the need to adopt advanced diffusion models for the correct description of flashback phenomena occurring in H2 flames.

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Ignition delay based estimation of laminar burning velocity as the minima of autoignitive reaction wave speed with unity Lewis number

Youhi Morii, Kaoru Maruta

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Understanding laminar flames is crucial for comprehending combustion phenomena. The laminar burning velocity, a key characteristic velocity of these flames, is recognized as an eigenvalue in the governing equations of one-dimensional flames. In this study, we present a novel approach to derive the laminar burning velocity. Our previously reported theory demonstrated that for a unity fuel Lewis number, the processes of zero-dimensional ignition and one-dimensional deflagration are equivalent. This equivalence is established through a spatio-temporal transformation, involving normalized temperature and fuel mass fraction, which represents the reaction's progress. Our theory posits that once a temperature is established, all related thermodynamic properties within the system can be determined, since temperature acts as a Legendre transformable function to these properties. Building on this, we discovered that the temperature gradient in one-dimensional deflagration is constrained by the profile of zero-dimensional ignition. Further, we found that this gradient is influenced by local velocity, which has an identifiable lower limit. We define this minimum velocity as the minima of autoignitive reaction wave speed. Consequently, this velocity is identified as the laminar burning velocity for a unity fuel Lewis number.

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Study on heat losses and flow rate on premixed hydrogen-air flame shape from thickness of Hele-Shaw burner

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The ability to accurately simulate flame propagation and predict flame instabilities for different gap sizes and equivalence ratios is crucial for the design of micro-scale combustion devices. In this work, numerical simulation based on a combination of the Lattice-Boltzmann method and detailed chemistry kinetic mechanism is carried out to recover stable premixed hydrogen-air flame front shapes on the thickness of a Hele-Shaw burner. Fundamental 2D flame shapes between narrow plates are computed by taking into account heat losses at the walls as well as the

flow rate ahead of flame front. Our numerical results successfully reproduce steady flame front shapes observed in experiments, all exhibiting convex profiles towards fresh gases over a wide range of equivalence ratio (from 0.35 to 2.0). The impact of equivalence ratios, gap sizes, heat losses and flow rate on flame shape symmetry/asymmetry properties have been investigated. Flame fronts tend to be more asymmetric then symmetric with increasing equivalence ratio. The range of symmetric flames narrows with increasing gap size. Additionally, both increases of heat losses and flow rate would widen the range of symmetric flames, hence it is essential to consider these two factors for the range of equivalence ratios where the transition from symmetry to asymmetry occurs.

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Multi-point optimization for laminar hydrogen flames

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Due to the increasing demand for high-efficiency and low-impact environmental technologies, hydrogen has become a prominent candidate to replace fossil fuels in combustion systems due to its lower emissions. However, as environmental regulations have become tighter, optimized combustion devices are required in order to meet these requirements. Therefore, this work presents developments in multi-point optimization for laminar hydrogen burners using the Discrete-Adjoint (DA) design framework within the multiphysics software suite SU2. The multi-point optimization is carried out in order to obtain a good balance between minimizing pollutant emissions and thermal efficiency over a range of equivalence ratios. The optimization cycle is driven using the open-source design optimization framework FADO. For combustion modeling, the flamelet generated manifold (FGM) approach, including preferential diffusion effects, is used. Using the FGM, the thermochemical properties are stored in lookup tables as functions of mixture fraction, enthalpy, and progress variable. For retrieving the information during simulations, artificial neural networks (ANNs) are used in order to replace the lookup tables and reduce computational requirements. These ANNs are trained using the open-source platform for machine learning TensorFlow. Finally, robust geometrical constraints will be shown, which allow to obtain optimized designs while preserving mesh quality along the DA-design cycle.

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Numerical Investigation on Flame Spread over a Thin Circular Duct

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The flame spread over combustible solids, such as cellulose paper, polymers, woods and textiles, constitutes a fundamental problem in the field of fire research. In the present study, flame spread over commonly encountered circular duct geometry is investigated numerically in normal gravity and microgravity environments.

A 2-D axi-symmetric numerical model is developed accounting for char formation to investigate the important mechanisms that controls the flame spread phenomena over circular duct geometry. In the present model the mass, momentum and energy conservation equations in gas phase are solved along with one-step, second order global gas phase reaction between fuel vapor and oxygen. In solid phase first order Arrhenius pyrolysis model is considered and mass and energy equation are solved in flame fixed coordinate system.

In the numerical investigation, it is found that radiation feedback from the char at inner core region of duct plays an important role on flame spread rate. Also, as the fuel radius increases the flame spread rate increases in the matrix of study.

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Track01-3 Laminar flames (3)

Chair: Youhi Morii
Friday, May 10; 09:50 - 11:50; Room M

Effect of confinement on the propagation patterns of lean hydrogen-air flames

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The effect of confinement on the propagation of lean hydrogen-air flames in a Hele-Shaw cell formed by two parallel plates separated by a small distance is studied numerically. Flame propagation is modeled using a quasi-three-dimensional (quasi-3D) approximation, where the momentum conservation equation is asymptotically reduced to Darcy's law. Chemistry is described by a one-step reduced kinetics with a simple model for transport properties. To assess the influence of momentum loss, comparisons are made with results obtained in an un-

confined geometry corresponding to a purely two-dimensional (2D) domain. Heat losses to the wall plates are also considered. The results demonstrate that momentum loss mainly increases the flame surface area by elongating the cellular structures in a finger-like form, with a relatively small enhancement of the reactivity at the flame front, consistent with a mechanism of hydrodynamic nature. This elongation leads to approximately a 50% increase in flame speed compared to the absence of confinement. Conversely, heat losses are observed to flatten the large-scale flame front and, if sufficiently large, can lead to the formation of isolated propagating two-headed flame cells or, ultimately, one-headed flame cells. The present results are well-aligned with recent experimental results.

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Effect of Taylor dispersion on triple flame propagation

Shumeng Xie[1], **Joel Daou**[2], Prabakaran Rajamanickam[2], Zheng Chen[1]
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Triple flames have been observed in non-premixed micro-combustion experiments, accompanying e.g. the formation of so-called diffusion-flame streets. In the present work, we identify the effect of Taylor dispersion or shear-enhanced diffusion on the propagation of such triple flames.

The study is carried out numerically within the thermo-diffusive approximation of constant density and transport properties and is based on a two-dimensional model derived asymptotically by depth-averaging the governing equations in a Hele-Shaw type configuration. The propagation speed of the triple flame, positive or negative, and its existence domain are determined in terms of three parameters, namely the Damköhler number, the fuel Lewis number and the Peclet number, with the latter quantifying the strength of Taylor dispersion.

It is found that Taylor dispersion significantly affects the propagation and existence domain of the triple flame, both directly through diffusion enhancement which thickens the flame leading-edge and modifies its curvature, and indirectly e.g. through the instability of the underlying diffusion-flame tail of the triple flame observed above critical values of the Lewis and Peclet numbers. In addition to the propagating and retreating triple flames, additional solutions are identified depending on the Lewis and Peclet numbers, including periodic flame arrays, and slowly-drifting isolated burning structures.

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Thermal Radiation Effects in Spherical Flame Simulations of Steam-diluted Hydrogen-Air Mixtures

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This study investigates the effect of thermal radiation on steam-diluted hydrogen-air flames. Steam dilution reduces flashback risks, temperature, and NOx emissions. These mixtures also impact nuclear safety, potentially arising in reactor cooling system breaches.

Prior studies using 1D simulations showed radiation (emission and reabsorption) significantly alters the laminar burning velocity (with observed accelerations exceeding 50% in realistic lean conditions). However, these models fall short in replicating experiments due to oversimplified geometry.

This research therefore shifts to 3D spherical flames, commonly used to measure laminar burning velocities experimentally. The goal is to match experimental results from a constant pressure spherical chamber using Direct Numerical Simulation coupled with a Monte Carlo radiation solver. This approach involves a two-way coupling between two 3D finite volume solvers. The combustion solver provides the temperature and composition, while the radiative solver returns the radiative power field. Special attention is paid to the compatibility of the different meshes and the adjustment of the coupling period to achieve the required accuracy. The aim is to accurately quantify radiation's impact and assess the precision of adiabatic fit models in predicting unstretched laminar burning velocities in lean and very lean hydrogen-air flames diluted with steam.

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Propagation and self-acceleration of circular expanding hydrogen/air flames at cryogenic temperature

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Hydrogen plays an important role in reducing carbon dioxide emission. The widespread use of hydrogen raises concerns on safety issues such as fires and explosions related to cryo-compressed hydrogen. Therefore, it is necessary to understand the combustion properties of hydrogen at cryogenic temperatures. In this study, we conduct two-dimensional simulations of circular expanding hydrogen/air flame in an open space and investigate the flame morphology evolution and self-acceleration process. Stoichiometric hydrogen/air mixtures with

near-unity Lewis number at cryogenic temperature (100 K) and normal temperature (300 K) are considered so that the flame propagation is mainly affected by the Darrieus-Landau instability (DLI) instead of the diffusional-thermal instability (DTI). Since the thermal expansion increases greatly with the decrease in the initial temperature, the DLI at cryogenic temperature becomes much stronger than that at normal temperature, which results in significant increase in flame propagation speed, total heat release rate, acceleration exponent as well as violent cell evolution including cell growth, splitting and merging. The stronger DLI at lower initial temperature leads to larger cell number, smaller mean cell size and longer mean cell depth. Analysis on cell statistics shows that the intermittent characteristics of flame propagation speed is mainly caused by cell evolution. Interestingly, the peak value of flame propagation speed at cryogenic temperature can exceed that at normal temperature. The heat release rate and flame propagation speed at cryogenic temperature can be comparable to those at normal temperature. Such counterintuitive observation provides useful insights to fire safety control of cryogenic hydrogen utilization.

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Numerical studies on the propagation of ultra-lean hydrogen/air flames in a narrow gap

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Understanding the propagation of ultra-lean hydrogen flame is important for hydrogen safety control. In this study, we conduct 3D numerical simulations on ultra-lean premixed hydrogen/air flame propagation in an open Hele-Shaw cells with conductive heat loss. By changing the wavenumber of perturbation imposed on the circular ignition kernel, effects of ignition kernel shape on flame cell propagation are studied. It is found that the ignition kernel shape significantly affects the flame cell evolution. When no perturbation is imposed on the circular ignition kernel, the smooth flame front splits into two isolated ball-like flame cells. These two flame cells propagate outwardly in one-headed finger regime. When the sinusoidal perturbation is imposed, flame front splits twice and forms four flame cells propagating outwardly in different flame regimes including one-headed finger and two-headed finger. The number of isolated flame cells is not sensitive to perturbation wavenumber. However, the distribution of flame cells as well as the interaction between adjacent cells is greatly affected by the perturbation wavenumber since it affects the isolated flame cells formation. Moreover, due to heat loss and counteraction of flame enhancement by positive stretch rate, the flame cell experiences periodic expanding and shrinking during its evolution. Furthermore, different flame cells tend to evolve into the same final state and the distance before reaching the final state is small when the isolated flame cell is far from adjacent cells. The present results help to understand the different regimes of ultra-lean hydrogen flame propagation.

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The propagation mechanism of laminar, premixed DME/air flames

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Dimethyl ether (CH3OCH3 or DME) is a bio-fuel that can be produced from renewable sources; e.g., liquefaction of biogas generated from fermentation processes. With the context of exploring its combustion characteristics, the propagation mechanism of DME/air steady, laminar, premixed flames is analyzed, using the tools of Computational Singular Perturbation (CSP). It is shown that this mechanism is encapsulated by an explosive mode, when it acts in a narrow region that includes the point where the maximum heat release rate (MHRR) occurs. The intense chemical activity downstream of MHRR generates heat and radicals that diffuse upstream, initiating chemical activity there that is sustained by the convective motion of DME and O2. The reaction contributing the most to the propagation mechanism is H+O2->OH+O, followed by other reactions that generate the radicals O, H and OH that are reactants of the most exothermic reactions (e.g., CH3+O->CH2O+H, CH2O+H->HCO+H, CH2O+OH->HCO+H2O). The species with the most impactful upstream diffusion is H, followed by OH and O that support the action of the explosive mode and of H2 that opposes it. The explosive mode is not everywhere meaningful; e.g., upstream of the flame, where transport dominates.

The proposed methodology carries out in an algorithmic manner the paper-and-pencil asymptotic analysis, introduced in the 80s by N. Peters, F.A. Williams and other researchers. However, being algorithmic, the CSP methodology is not hindered by the size of the kinetics mechanism or the complexity of the reacting configuration employed.

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Track01-4 Laminar flames (4)

Chair: Ekenechukwu Chijioke Okafor
Friday, May 10; 13:00 - 15:00; Room M

Effect of Ozone Addition on Extinction limits of Hydrogen/Ammonia-Air Premixed Counterflow Flames

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Effects of Ozone addition on enhanced reactivity leading to increased flame speed, ignition limits and achieving cool flames has been reported in literature. However, studies on the impact on flame extinction limits in case of strained flames are relatively scarce. Extinction resistance of flame due to stretch is an important property for understanding combustion behaviour in turbulent flows as well as for chemistry tabulation. The present study investigates the effects of ozone addition on the extinction of strained hydrogen/oxygen/nitrogen and ammonia/oxygen/nitrogen flames, emphasising change flame structure due to the chemical kinetics of ozone. A twin premixed flame, symmetrical about stagnation plane and a single premixed flame opposing inert nitrogen are studied computationally using the counterflow flame configuration. The addition of ozone in oxidizer further promotes the reactions by generating the radical pool of O, OH, HNO, NO, etc. especially for lean mixtures, which show significantly higher extinction stain rates (ESR) than those without ozone. This is predominantly due to the additional ozone layer in the preheat zone also manifesting as dual peaks in heat release rate profile. However, the ozone addition has a limited effect on rich mixtures. In the case of ammonia, although HNO production is significant on the rich side, limited O, OH, and NO radicals suppress the further chain branching through NH2, NH, etc. The flames with different burner separation distances (BSD) are also studied to further the understanding of apparatus independent ESR and its use in the validation of kinetic models.

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Optimized Progress variable for methane-hydrogen flames

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In the context of gas turbines, the turbulent burning speed is strongly influenced by the laminar burning speed, which is directly tied to the type of fuel being used. When a portion of methane fuel is replaced with hydrogen, it has a significant impact on the chemical processes involved. This not only affects the rate at which fuel is consumed but also has implications for flame stability, potentially leading to higher integral fuel consumption rates. When considering a non-unity Lewis number for fuels that include hydrogen, there are localized variations in the distribution of species and temperature. These localized changes have an effect on the local consumption rate of fuel, which can result in an unstable flame. To study this phenomenon, the flamelet model is employed, which represents flames as a collection of one-dimensional laminar flames. , and a genetic algorithm is used to optimize the progress variable by minimizing non-monotonicity terms and the gradient of species concentrations.

By constructing flamelet tables with a non-unity Lewis number and introducing hydrogen into methane fuel, different progress variables are compared. The findings highlight the significant influence of certain chemical species on the progress variable and demonstrate the sensitivity of the defined cost function to the selected species, particularly when there is an increase in the amount of hydrogen in the fuel. It is crucial to include CO in the progress variable definition to accurately represent the combustion process.

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Estimating Soot Formation/Oxidation Rates using Explainable Machine Learning

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Soot, the second most significant contributor to climate change following CO2, has detrimental effects on the environment and human health. Understanding soot formation and oxidation is crucial for mitigating the environmental impacts of hydrocarbon combustion. Numerical modeling of soot formation requires considerable computational resources and time due to its dependence on numerous physical and chemical processes, entailing the integration of thermodynamics, heat transfer, chemical kinetics, particle dynamics, and fluid dynamics. A key goal of the combustion industries is to develop accurate and computationally inexpensive approaches for obtaining soot properties. This study investigates the application of Explainable Machine Learning (XML) to estimate soot formation/oxidation rates by employing the histories of correlated gas-related variables, such as temperature, mixture fraction, and species concentrations. The current work finds the complex relation between input features and soot formation/oxidation rates and provides transpar-

ent insights into the ML algorithm's decision-making process. The approach aids in gaining a deeper understanding of the physical aspects involved in soot formation with lower computational costs compared to CFD simulations. Prediction accuracy is tested over two segregated flames, having an R2 value of approximately 0.87.

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Numerical Study of Co-combustion Characteristics of Ammonia and Coke Oven Gas

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This study numerically investigates the co-combustion of ammonia with coke oven gas (COG) that is produced during the manufacture of metallurgical coke. Chemkin-Pro 2020 R1 software with a detailed chemical mechanism is used to predict adiabatic, freely propagating laminar burning velocities for NH3/COG combustion. Ammonia is a new type of carbon-free fuel and has the advantage of easy transport. However, ammonia combustion has some defects, such as a high ignition temperature, low flame temperature, slow flame speed, and narrow range of flammability. COG, abundant in hydrogen, possesses a substantial energy content and can effectively address the limitations associated with ammonia combustion.

Co-combustion strategy synergizes the advantages of both fuels, aiming to maximize their potential and achieve carbon reduction benefits. By delving into the fundamental flame properties and pollution emission characteristics, a detailed analysis will be performed for the combustion kinetics and thermodynamics of the co-combustion system. Furthermore, the study will also explore combustion characteristics of NH3/COG-air premixed flames including adiabatic flame temperature, flame velocity, flame structure, and species distribution. The results will contribute to the development of a novel combustion technology with potential environmental benefits, simultaneously improving the utilization efficiency of both ammonia and COG.

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Numerical Study on Hydrogen Peroxide Effect on Syngas/Air Premixed Combustion

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Synthetic gas (syngas), derived from biomass gasification, is a promising fuel source and is mainly composed of hydrogen and carbon monoxide. However, syngas is usually categorized as a low-caloric fuel that needs to be enhanced for various combustion applications. Typically, syngas combustion can be enhanced by adding a strong oxidant, such as hydrogen peroxide. Hydrogen peroxide (H2O2) is a strong oxidizer that yields oxygen, steam, and appreciable heat after decomposition. Adding hydrogen peroxide to syngas combustion can significantly enhance the potential of syngas through chemical modifications. Different roles of H2O2 in syngas/air combustion can be leveraged to realize its advantages. These roles include treating H2O2 as a fuel addition, an oxidizer addition, and an oxygen replacement in air. This study numerically investigates the effects of H2O2 on syngas/air-premixed combustion by varying the H2O2 addition method using the CANTERA package combined with a detailed chemical mechanism. The adiabatic flame temperature, laminar burning velocity, flame structures, and some major species evolution for one-dimensional simulation are discussed under different simulation conditions. The results will contribute to the development of syngas as a promising fuel with potential environmental benefits, simultaneously improving the utilization efficiency.

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Track01-5 Laminar flames (5)

Chair: TBD
Friday, May 10; 15:20 - 17:20; Room M

Regimes of autoignitive stretched flame bounded by "Explosive transition of deflagration" and spontaneous ignition front

Akira Tsunoda, Youhi Morii, Kaoru Maruta
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To enhance thermal efficiency and lower emissions, advanced engine technologies like HCCI are gaining focus. These operate in extreme conditions like high temperature and pressure, posing challenges such as knocking. Traditional laminar deflagration theory, which separates

deflagration into preheat and reaction zones, does not fully explain these phenomena. This study examines deflagration limits at elevated temperatures, introducing concepts of "Explosive transition of deflagration" theory, the limit of deflagration with Lewis number greater than unity (Le > 1) caused by chemical reactions in the preheat zone, and "spontaneous ignition front", represented by the characteristic speed in temperature-inhomogeneous mixtures proposed by Zel'dovich. The study confirmed equivalency between 0D ignition and 1D counterflow flame (stretched flame) with Le = 1, applying this to numerical simulations of 1D stretch-free and stretched flames for Le > 1. 1D stretched flames showed three reaction front regimes with increasing mixture temperature: (I) conventional deflagration, (II) deflagration affected by spontaneous ignition in the preheat zone, and (III) spontaneous ignition front. "Explosive transition of deflagration" of 1D stretch-free flame was observed in the vicinity of the boundary between the regimes (I) and (II). Regime (III)'s phenomena aligned with Zel'dovich's spontaneous ignition front theory.

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Evaluation of Soret Diffusion Models for Hydrogen Combustion

Thorsten Zirwes, Andreas Kronenburg
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Hydrogen is becoming increasingly important as a zero-carbon fuel. However, hydrogen is characterized by strong differential diffusion effects due to its high diffusivity. This not only affects Fickian diffusion (non-unity Lewis number effects), but an additional mass flux due to thermodiffusion (Soret effect) becomes important as well. The most accurate approach currently is to compute thermodiffusion coefficients from the multi-component diffusion model. However, the computational cost for the multi-component diffusion model is prohibitively large when performing full 3D simulations of hydrogen flames. In this work, we implemented five different approximate diffusion models from the literature and directly compared them to the multi-component diffusion model. These include models available in commercial codes like Fluent and Chemkin, in-house codes and the literature. The model by Warnatz et al. yields the best results for thermodiffusion coefficients of the light species H and H2, but prediction of heavier species shows significant differences. Overall, the model by Chapman and Cowling performs the best, while other commonly used models show large discrepancies to the multi-component reference values. The best model is then used to perform a full 3D simulation of a thermodiffusively unstable hydrogen flame to study the formation of cellular structures.

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Numerical investigation of a water droplet interacting with an hydrogen/air counterflow flame

Maria Rosaria Acquaviva, Biagio Cassese, Alessandro Porcarelli, Ivan Langella
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The mutual interaction between a single water droplet and a strained laminar premixed hydrogen-air flame is numerically investigated in this work. The topic is relevant because the injection of water droplets is emerging as a possible solution to lower NOx emissions in premixed combustion systems. Indeed, the water vapor located close to the flame absorbs heat with a consequent reduction of temperature, thermal NOx, and the possible control of temperature fluctuations. However, for common hydrocarbon fuels the process of water droplet evaporation near the flame might lead to local extinction with consequent increasing of CO emissions. Conversely, the strong reactivity of hydrogen can prevent the occurrence of local extinction when the injected droplets reach the flame front, which makes water injection very attractive for hydrogen flames. Together with this, the vapour cloud forming around the droplets during the evaporation process might induce a local wrinkling of the flame front with consequently local curvature effects which are particularly important in lean hydrogen flames due to the high diffusivity of hydrogen. These effects are studied in this work by means of two dimensional detailed chemistry simulations, specifically focusing on the local interaction between strain and the local curvature induced by the droplet-flame interaction.

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Nozzle Angle Effect on Premixed Conical Flame-Flickering Characteristics

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Experimental and numerical simulation methods were utilized to investigate the impact of nozzle angle on the characteristics of premixed conical flame flickering. This study specifically examined a typical premixed conical flame (Bunsen flame) across a range of nozzle directions from 0° to 180°. A notable aspect of this research is the comprehensive collection of flame flickering frequency data obtained through heat release signal experiments.

While the flickering frequencies exhibit a consistent influence from equivalence ratio and Reynolds number, their distribution varies across different nozzle angles. The research also presents a novel empirical correlation for general nozzle angles based on the collected data. To provide clearer insights into flame behavior under varying nozzle angles, velocity fields were visualized using Particle Image Velocimetry (PIV) experiments and Direct Numerical Simulation (DNS). The results indicate that the nozzle angle not only alters downstream shear strength but also affects general flame flickering and vortex shedding motions.

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Three-dimensional simulations of ultra-lean hydrogen-air flames in narrow gaps

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Motivated by recent experimental evidence demonstrating the stationary propagation of isolated flame cells in ultra-lean mixtures containing hydrogen and air between two parallel plates, this work conducts a three-dimensional study to numerically explore the transition between the double-cell and the circular flame solution in relation to the equivalence ratio. The chemistry is described by a one-step reduced kinetics, previously developed for hydrogen-air deflagration, along with a simple model for the transport properties. The separation distance between the plates is fixed at 4 mm. Additionally, the impact of heat loss through the walls on the development of each flame solution is examined. The simulations reveal propagation velocities and sizes of isolated flame cell solutions consistent with the experimental observations.

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Numerical Investigation of micro-combustion flame dynamics on wavy systems: materials and performance analysis

David D. Dias[1], Pedro Resende[2], **Alexandre M. Afonso**[3]

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The increasing demand on combustion based micro-power generation systems, mainly due to the high energy density of hydrocarbon fuels, created a great opportunity to develop portable power devices, which can be applied on micro unmanned aerial vehicles, micro-satellite thrusters, or micro chemical reactors and sensors This work studies numerically micro-combustion to design micro-propulsion, which can be applied on micro unmanned aerial vehicles or CubeSat. For these numerical studies we use a numerical framework for the numerical modeling of laminar flows with homogeneous reactions and analyze heat transfer within the solid walls of the microchannel using the Conjugate Heat Transfer method. The implementation was fully validated with numerical and experimental studies.

In this work, we conduct a numerical study of flame dynamics in complex geometries, exploring the impact of various materials commonly used in aerospace applications on propulsion. By adjusting input parameters and operational conditions, we aim to understand how different materials affect the design and performance of the micro-burner systems. We examine five material groups, including adiabatic materials, ceramics (LTCC and HTCC), metals (two stainless steels), amorphous materials (two high-temperature glasses), and high thermal conductivity materials (silicon, aluminum, and copper-tungsten alloys).

A new type of flame dynamics for Hydrogen/air combustion were observed, named Pulsatory Flame Burst (PFB) [1-6]. The phenomenon known as Pulsatory Flame Burst (PFB) is a specific flame behavior characterized by burst-like flame pulsation due to flow and combustion interactions. As of currently, PFB only occurs in undulating geometries with premixed hydrogen and air, and the flame bursts involve the ignition, propagation, bifurcation (splitting), and extinction of the flame in a cyclic manner. This new type of flame dynamics can be explored to design new efficient and compact green energy burner due to the extended limit for flammability introduced by the interplay between fluid dynamics and combustion, particularly due to the vortices generated on the nonlinear geometry of the burner.

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Track02 Kinetics, mechanism reduction

Track02-1 Kinetics, mechanism reduction (1)

Chair: Maria U. Alzueta
Wednesday, May 8; 15:30 - 17:10; Room K

Deep mechanism reduction (DeePMR) method for fuel chemical kinetics

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Fuel chemistry represents a typical complex system involving thousands of intermediate species and elementary reactions. Traditional mechanism reduction methods, such as sensitivity analysis and graph-based approaches, fail to explore global correlations of the sub-systems, thereby compromising their efficiency and accuracy. A novel machine learning-based approach called deep mechanism reduction (DeePMR) has been developed to address this issue. The current method transforms mechanism reduction into an optimization problem in the combinatorial space of chemical species while mitigating the curse of dimensionality inherent in the high-dimensional space. We propose an iterative sampling-training-predicting strategy combining deep neural networks with genetic algorithms to learn the landscape of the combinatorial space and locate the targeted subspace. Applying DeePMR to fuel chemistry mechanisms has led to much more compact mechanisms than traditional methods, including directed relation graph (DRG) or path flux analysis (PFA) methods, with three to four orders of magnitude acceleration in numerical simulation. In addition, reduced mechanisms by DeePMR indicate a principal-satellite formulation for constructing chemical reaction mechanisms, providing a straightforward yet effective alternative to hierarchy-based construction methods. The DeePMR method provides a general framework for model reduction across various fields.

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An open-source toolbox for chemical kinetic mechanism's optimization

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In the field of chemical kinetics, optimizing kinetic mechanisms is highly important for more accurate simulations and predictions. This study introduces a novel and open-source toolbox based on JAYA optimization algorithm. JAYA has already proven its capabilities in many engineering problems, and in this study, it is utilized for the first time in the field of chemical kinetic mechanism optimization. The toolbox uses Cantera for solving chemistry related computations, ensuring robust and reliable results. A notable feature of this toolbox is its user-friendly Graphical User Interface (GUI), developed in a Python environment. This GUI simplifies the optimization process and, with its open-source nature, is accessible to a wider range of users. It enables users to conduct sensitivity analysis and define the uncertainty ranges of Arrhenius rates, which are crucial for fine-tuning mechanisms. The toolbox is capable of optimizing three combustion parameters such as ignition delay times, laminar burning velocities, and jet-stirred reactor mole fractions. Additionally, by using "multiprocessing" library, each data point can be evaluated on different processors, which helps in reducing the overall computational time. After numerous test runs, the results have been satisfactory, demonstrating the toolbox's capability to effectively and accurately optimize chemical kinetic mechanisms.

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Combined chemical reaction network and time scale analyses for reduced models of combustion of complex fuels

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Chemical reaction networks (CRNs) of combustion systems based on mass action laws and Arrhenius reaction rates of elementary reactions remain the primary sources for complexity of the combustion models. A number of

variables / species and parameters used as well as stiffness of models complicates significantly the computational treatment considerably. This becomes even more crucial once a mixture of different fuels is considered.

In this work, we use a combination of time scale, invariant manifolds and chemical reaction network analyses to study ignition delay times of combustion systems of complex fuels. The blends of hydrogen, methane mixed with ammonia as combustible systems are considered. Rigorous time scale analysis of detailed model and study the CRN properties, while varying the composition, identifies the rate limiting and coupled sub-networks controlling the ignition delay times and describing the course of combustion system dynamics. As a results key reactions controlling the progress and constraining the states are identified, which can be used to both improve the detailed models as well as to reduce detailed chemical reaction models.

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Minimizing Reduced Mechanism Costs via Bounded Reaction Rate Optimization and Targeted Reaction State Sampling for Engineering Applications

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Finite rate chemistry is a computationally expensive component of many numerical simulations of combustion applications. With significantly lower computational cost compared to detailed chemical mechanisms, reduced mechanisms employing the quasi-steady state approximation (QSSA) typically reproduce key combustion responses with high accuracy. However, simulation costs with reduced mechanisms are still significantly higher than those with global mechanisms. To lower costs while maintaining accuracy sufficient for engineering applications, two ideas are considered: 1) optimization of reaction rates within uncertainty bounds and 2) reduction at targeted sets of conditions corresponding to a single combustor operating point. Reduction costs are low relative to numerical simulations of applications, so a unique mechanism can be created for each operating point with minimal impact on computational budgets. Recently presented work on novel skeletal mechanisms derived from this approach demonstrates cost-savings that range from marginal to 50% relative to skeletal mechanisms in the literature, and in cases where cost-savings are marginal, order of magnitude reductions in ignition delay errors are observed. In this presentation, the QSSA is applied to these novel skeletal mechanisms to yield novel reduced mechanisms; cost and accuracy improvements are then considered relative to existing reduced mechanisms. Cost assessments include comparisons of chemical timescale estimates and associated time step restrictions for numerical simulation of applications.

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NH3/DME oxidation at different pressures

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The present study deals with the conversion of NH3/DME mixtures in tubular flow reactor setups at different pressures, ranging from atmospheric to 40 bar. The experimental work includes variation of temperature (500-1425 K), O2 excess ratio (λ= 0-3), NH3/DME ratio (0.5-10) and pressure (up to 40 bar). Additionally, the influence of the impact of the presence of NO has also been considered at atmospheric pressure. The results show that the presence of DME affects the oxidation behavior of NH3, displacing its oxidation at low temperatures. This effect increases as DME concentration increases. O2 availability and pressure influence significantly the conversion of both components of the mixture, shifting it to lower temperatures as O2 excess ratio and pressure increase. Similar effect is produced by the presence of NO, except for DME oxidation, which is only enhanced under fuel-lean conditions in the presence of NO. Pressure also acts to increase N2O production. Simulation of the experimental results has been done using different mechanisms and results indicate that varying pressure implies significant differences in both experimental results and reaction pathways.

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Track02-2 Kinetics, mechanism reduction (2)

Chair: TBD
Friday, May 10; 09:50 - 11:50; Room E

Development of a Kinetic Mechanism for Ammonia blended Combustion Applications in CI Engines and Gas Turbines

Sayak Banerjee, Raja Banerjee, Dinesh Prabhakaran
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Ammonia (NH3) is considered a promising carrier of renewable hydrogen and a zero-carbon fuel. Despite its many advantages, ammonia does suffer from poorer combustion characteristics compared to traditional hydrocarbons like lower flame speeds, high ignition delay times and high NOx formation propensity. Hence ammonia must be used in blended form with other traditional fuel molecules like Methane, Kerosene and Diesel in dual fuel CI engines or Gas Turbine applications, at least at the initial stages. The current work is aimed at constructing a semi-detailed ammonia – methane – hydrogen – n-dodecane mechanism consisting of 242 species and 1769 reactions including both nitrogen oxides (NOx) and soot sub-mechanisms to investigate the combustion and emission characteristics of potential blends of ammonia with traditional fuels in emerging gas turbine and CI engine systems. The ignition delay and laminar flame properties of the fuels and their blends have been predicted using this mechanism and validated extensively with numerical or experimental data available in the literature. Some initial combustion and emission characteristics of promising blends are also discussed.

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A skeletal chemical kinetic mechanism for ammonia-kerosene oxidation in air

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The immediate transition of kerosene-based gas turbine engines towards sustainable energy generation can be achieved through the adoption of ammonia-kerosene blends combustion. In addition, the slow combustion kinetics of ammonia can be addressed by burning it with higher reactivity fuels like kerosene. It is essential to develop ammonia-kerosene mechanisms to grasp the impact of adding ammonia on the combustion characteristics and emission features of kerosene-based fuels. In the present work, ammonia-kerosene skeletal chemical kinetic mechanism is developed using the decoupling methodology to avoid conflicts in rate constants for identical reactions while merging mechanisms. The present mechanism includes four subsets: ammonia subset, kerosene subset, O2/H2 subset, C1/NOX/NHi subset. The ammonia subset with N/O/H reactions is taken from Okafor mechanism meant for NH3/CH4 oxidation in air. The kerosene subset with C/O/H reactions along with the O2/H2 subset is taken from Zettervall mechanism meant for Jet A-1 oxidation in air. The C1/NOX/NHi subset is adopted from Okafor mechanism as coupling reactions between nitrogen and carbon primarily rely on interactions involving small radicals in high-temperature chemistry. The reaction rate constants of different subsets are updated from several mechanisms from the literature based on flame speed and OH sensitivity analyses. The newly proposed mechanism demonstrated close validation of laminar burning velocity and ignition delay values with the experimental data at different pressures, temperatures, and equivalence ratios for neat fuels owing to the lack of data related to the blends.

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Developing an Ionic Mechanism for Numerical Modeling of Ion Currents in Ammonia-Air Flames

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With the advent of ammonia-air combustors, diagnosing the state of combustion within these devices becomes necessary. As with hydrocarbon flames, ammonia-air flames possess a measurable ion current and a relationship between the equivalence ratio of the ammonia fuel-air mixture and this ion current is seen to exist. In laminar stagnated flame experiments, this relationship is quite straight forward with the ion current peaking in the lean zone just shy of stoichiometry and falling off either side of this. However, in complex combustors such as swirl burners, what can be described as a "spatial ion current map" is observed. In order to understand the phenomena responsible for the complex ion currents observed in combustors, numerical modelling becomes a necessity. Arguably the most important component in this numerical modeling process is the reaction mechanism. While several reaction mechanisms exist for ammonia-air combustion, an ionic reaction mechanism did not exist prior to this

research endeavor. This study details the path taken in developing the ionic mechanism, how well it corroborates experimental findings, its application in chemical kinetics based numerical simulations, some peculiarities of applications in these models, and aspects of the mechanism that require further improvement.

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Simplified chemical reaction model and its application in combustion and detonation

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The simplified model of REDIM was established according to the experimental parameters and boundary conditions in this paper . By comparing the relationship between the CO2 generation rate and its mass fraction in the developed REDIM model and the same relationship diagram in the single-step method and the primitive method, the validity of the REDIM model is verified. The N-S equation considering viscous diffusion and heat conduction is established, and the LES control equation is obtained by spatial filtering of the N-S equation. The flame surface density model is used in the single-step reaction model and the elementary reaction model. In the REDIM model, the flame surface density model is combined with the REDIM method to generate a manifold to form a new combustion model. A numerical simulation calculation program capable of simulating the whole process of combustible gas flame acceleration and DDT was prepared. Large eddy numerical simulations were carried out using three chemically simplified reaction models (one-step reaction model, 14-component 19-step elementary reaction model and REDIM model) for experiments of DDT in small-scale pipeline and the scenario that DDT doesn't happen in small-scale pipeline. By comparing with the experimental results, the accuracy of the numerical simulation results of the REDIM model is verified.

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Track02-3 Kinetics, mechanism reduction (3)

Chair: Akira Miyoshi
Friday, May 10; 13:00 - 15:00; Room J

On the kinetics of oxidation of n-butane at high-pressure

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The autoxidation of n-butane was studied experimentally in a jet-stirred reactor at 10 atm over a range of temperatures (530-1030 K) and equivalence ratios (0.25, 1, and 1.5). Products of oxidation were analyzed in the gas phase by gas chromatography using several detectors (Flame ionization detector, thermal conductivity detector, quadrupole mass spectrometer), hydrogen peroxide analyzer, and Fourier transform infrared spectroscopy. Besides the n-butane and oxygen, 38 products were quantified. Kinetic modeling was performed using a kinetic reaction mechanism already used to simulate previous n-butane oxidation experiments in the cool-flame regime. Although improvements are needed to better describe the oxidation of n-butane under the present conditions, the model represents the major trends of n-butane oxidation. A kinetic analysis indicated the major reaction pathways to products and the sensitive reactions.

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Effect of Oxygen Enrichment on the Combustion and Emission Characteristics of Premixed n-Butane/Air Flames

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The numerical investigation is carried out on laminar premixed n-butane/air mixtures enriched with oxygen, with the range of enrichment factors varying from 0 to 0.79 for lean (φ = 0.8), stoichiometric (φ = 1.0), and rich (φ = 1.2) mixtures, respectively. The role of oxygen enrichment on combustion characteristics is thoroughly investigated by comparing its major global thermal properties and emissions using a detailed kinetic mechanism with 67 species and 475 elementary reactions. Oxygen enrichment increases the overall heat release rates, flame speed, adiabatic flame temperature, and reaction zone temperature. A gradual decrease in flame thickness is observed

with increasing O2 enrichment. The rate of increment in flame speed is more predominant in the range of oxygen enrichment factor of β = 0-0.4, with respect to the higher range of β = 0.5-0.79 for all the cases of equivalence ratio, φ. The peak value of the heat release rate of the stoichiometric n-butane/air mixture increases by about 20.9% and 48.5% for the enrichment factors, β = 0.4 and β = 0.79, respectively. The CO emission index indicates a linearly increasing trend with increasing O2 enrichment, while the NOx emission index portrays parabolic dependence with an increase in O2 enrichment. The outcome of the present work can be implemented as the fundamental database for CFD modelling of oxygen-enriched combustion for the different hydrocarbons using DNS/LES modelling in real-time combustion applications.

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Reduced models for the methane-hydrogen air systems using Reaction Diffusion Manifolds accounting for differential diffusion

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The description of differential diffusion, particularly in blended fuels, has always presented a challenging problem in manifold-based model reduction. In blended fuel mixtures, modelling diffusion coupled with reduced kinetics is a challenging task. In addition, considerable care is needed when using manifolds for the reduced system integration, because system states that may evolve away from the manifold due to diffusion processes have to be relaxed back onto the slow manifold which is both invariant and attractive.

In this talk, a generic approach to treat differential diffusion effects in manifold based reduced models is presented. To define a reduced system of equations, the terms in the governing equation are projected onto the slow manifold in local coordinates. The net rate of movement along the manifold then describes the evolution of the system according to the slow processes. In addition, it is shown that usage of generalized coordinates to describe the manifold and integrate the system equations increases the robustness of the method considerably.

The approach is applied to Reaction Diffusion Manifolds (REDIMs) for premixed methane-hydrogen-air mixtures in freely propagating flames. The variation of flame-speed with change in hydrogen content in the mixture is computed and used to validate the reduced model.

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A ethanol reduced mechanism using real gas equation of state and its application in virtual chemistry

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Numerous studies have explored methods to decrease particulate emissions from vehicle exhaust gas, significantly contributing to air pollution in urban areas. One approach with promising potential is supercritical combustion, which involves injecting fuel over its critical temperature and pressure. Supercritical fluids have a lower viscosity and surface tension than liquids and a higher diffusion rate, leading to a more uniform mixture distribution that enhances thermal efficiency and reduces particulate emissions. This study focuses on using supercritical ethanol as a biofuel option, proposing a reduced kinetic mechanism comprised of 71 species and 684 reactions obtained through directed relation graph error propagation and sensitivity analysis. They validated this mechanism using Cantera with a cubic Redlich-Kwong and an ideal equation of state for constant-volume auto-ignition delay time and laminar flame speed simulations for pure ethanol. The IDT results are consistent with experimental data at 10, 30, 50, 75, and 80 atm in a temperature range of 700 - 1250 K, showing a satisfactory agreement with LFS experiments at 380 - 400 K, 1 - 4 atm and (ϕ) of 0.6 - 1.4.

A two-step virtual chemistry optimized mechanism is derived from the developed ethanol mechanism to provide a mechanism suitable for high-fidelity applications. The real chemistry mechanism was used to create the learning database and the virtual mechanism to reproduce the evolution of the laminar flame speed and temperature profiles of a one-dimensional freely propagating laminar premixed flame with the equivalence ratio for the ethanol/air flame at 394 K and 1 atm.

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A two-step virtual optimized kinetic mechanism for butanol from a newly developed detailed mechanism for alcohol fuels

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The efficient use of energy resources and climate change are important concerns in contemporary society. So, the search for biomass-based renewable fuels have

increased. Among the second generation biofuels, alcohol fuels have many advantages and n-butanol has better properties when compared to ethanol, such as higher heating value and lower saturation pressure. To fully understand these fuels, a comprehensive description of the reaction pathways and high fidelity computational studies are needed. The level of description of detailed mechanisms is usually prohibitive when dealing with high fidelity simulation. To overcome the computational cost, numerical stability and modelling issues, chemical mechanism reduction techniques must be applied. The virtual chemistry uses machine learning to derive a virtual mechanism from a detailed database. Using a genetic algorithm, a two-step virtual mechanism composed of a few virtual species capable of capture the flame structure while mimetizing mixture-averaged targeted quantities of the real compound is derived from scratch. However, the virtual mechanism does not model real reactions and species and the virtual reactions and virtual species may be understood as a mathematical tool calibrated to mimetize the targeted quantities. The present work presents a newly developed detailed mechanism for alcohol fuels using the demi-decoupling methodology. Furthermore, the detailed mechanism is used to construct the learning database for virtual chemistry and a two-step virtual mechanism for butanol is derived. The specific heat capacity at constant pressure and specific standard enthalpy of formation of the burnt gases and laminar flame speed and temperature profiles are defined as target.

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Track03 Ignition, quenching

Track03 Ignition, quenching

Chair: Debojit Sharma
Thursday, May 9; 09:50 - 12:30; Room C

Numerical investigation of spark ignition processes of NH3-H2-air mixtures in a laminar strained premixed configuration

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Understanding the ignition properties of ammonia / hydrogen /air mixtures is essential because of their abundance in chemical engineering processes, and their prospective role as fuels in future energy systems. This work investigates ignition processes of ammonia/hydrogen/air laminar strained premixed flame configurations by numerical simulations. These track the evolution of ammonia/hydrogen/air mixtures during and after the deposition of ignition energy, using a detailed treatment of chemical reactions and molecular transport . Studies on the influence of different parameters on the minimally required ignition energy are performed. These are the strain rate, hydrogen content in the fuel, pressure and initial (pre-ignition) temperature. Analysis of the results supports a knowledge-driven approach to the development of fail-safe ignition devices and to a reliable prevention of explosion hazards. The simulations are used for evaluating the ignitability of ammonia and its mixtures with hydrogen.

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Numerical Investigation on Quenching Distance of Laminar Premixed Methane/Hydrogen-Air Flames

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The transition from natural gas to hydrogen has been escalating in recent years. Fully hydrogen-fuelled burners, both at the industrial and domestic scales, have gained attention. To facilitate this transition, an understanding of flashback and quenching behaviour becomes crucial. In this study, the flashback and quenching behaviour of laminar premixed flames is modelled in two dimensions with detailed chemistry. Quenching distances are determined by initially modelling a stable flame and then abruptly decreasing the inlet speed of the mixture, enabling upstream propagation of the flame in a converging duct. The quenching distance is defined as diameter at the point where the flame extinguishes, mainly due to the heat loss from the flame to the wall. The obtained results for methane and hydrogen-air mixtures at various equivalence ratios are compared with experiments from the literature, demonstrating good agreement. The effect of premixture inlet speed on quenching diameter is investigated, revealing that the quenching diameter decreases with decreasing inlet speed. The variations in quenching diameter across different geometries, such as slit, circular duct, or annular duct, are also discussed in this work. Additionally, the effect of wall temperature on quenching distance is explored, revealing that quenching distance decreases with increasing wall temperature.

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Effects of Wall Heat Transfer Properties on Head-on Quenching of Hydrogen/Air Flames

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This study explores the impact of wall heat transfer on the head-on quenching behavior of hydrogen/air flames. Numerical simulations of one-dimensional laminar flames were conducted using chtMultiRegionFoam of OpenFOAM v10. The solver uses (i) conjugate heat transfer, (ii) mixture-averaged diffusion model, and (iii) the Wang-2018 mechanism. In order to quantify the wall heat transfer effects, three wall thermal conditions including (i) adiabatic, (ii) isothermal, and (iii) conjugate heat transfer were considered. For the conjugate heat transfer wall, a wide range of thermal conductivity and volumetric heat capacity of the wall were explored to observe the head-on quenching distance and heat loss to the wall. The findings indicate

that an increase in thermal conductivity and volumetric heat capacity leads to higher heat loss through the wall and an extended head-on quenching distance. Future work aims to identify key relationships that can parameterize the quenching behaviors from adiabatic to isothermal wall conditions. Additionally, a predictive model will be proposed to quantify the head-on quenching distance and heat loss based on the thermal properties of the wall.

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Numerical Study of Hydrogen Enrichment Effects on Methane/Air Flame Propagation in Crevices

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The propagation of premixed flames in narrow channels/enclosures is a typical problem encountered in combustion devices. In internal combustion gas engines, it has been speculated in the past that large proportion of the unburned hydrocarbon emissions may originate from the flow of unburned fuel through the gap between the piston rings and the cylinder wall. Due to the large surface-to-volume ratio, a premixed flame may rapidly quench upon propagating through the crevice and interacting with its walls, hence the accumulation of unburned hydrocarbons. This scenario could be possibly alleviated by increasing the mixture burning velocity through hydrogen enrichment. In the present study, we investigate a 2D model problem of a premixed flame approaching a narrow enclosure with cool walls at different channel heights and methane/hydrogen ratios at atmospheric conditions. We utilize direct numerical simulations and a finite rate chemistry solver in the OpenFOAM framework. We observe that both adding hydrogen to methane/air mixture up to 60% (molar) percent of the fuel mixture, as well as increasing the crevice height may both individually promote the flame propagation to the end of the crevice, hence considerable reduction of the unburned hydrocarbons in the system.

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DNS of forced ignition and flame-edge dynamics in turbulent ammonia/hydrogen/air and methane/air mixing layers

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Ammonia (NH3) is a promising zero-carbon fuel because of its mature manufacture, reliable large-scale storage and convenience in transport. However, the ignition of ammonia/air mixture in practical combustion engines is challenging due to the low reactivity of ammonia. Blending ammonia with hydrogen can improve the reactivity of the fuel mixture, and promote the ignition process. In the present work, the ignition and combustion characteristics of ammonia/hydrogen and the commonly used hydrocarbon fuel, i.e. methane, are investigated. In particular, forced ignitions in turbulent ammonia/hydrogen/air and methane/air mixing layers are studied using three-dimensional direct numerical simulation (DNS) with detail chemistry, and the aim is to investigate the ignition process and flame-edge dynamics of ammonia/hydrogen/air and methane/air mixtures. The general characteristics of the forced ignition process are analyzed and compared for various cases, with a particular focus on the heat release rate and temperature distributions. The flame edges are identified. The flame-edge speed and its components are compared for various cases and the correlation between the flame-edge speed and scalar dissipation rate is examined.

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Large-Eddy Simulations for spark-ignition of lean H2/air mixtures using a stretch-adapted Thickened Flame Model

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Lean hydrogen-air combustion is gaining interest in the context of the energy transition towards decarbonized fuels. Our study aims to simulate the spark ignition of a lean H2/air mixture using the Thickened Flame Model (TFM) with adapted flame response to stretch. The TFM is a turbulent combustion model for Large Eddy Simulations (LES) widely used in industrial and academic studies [1]. In prior studies, the TFM was coupled with Adaptive Mesh Refinement (AMR) to reduce computational costs while directly resolving chemical reactions on LES grids [2]. The TFM ensures the preservation of the laminar flame speed. However, it is well known that the standard TFM leads to erroneous modification of flame speed and structure

due to stretch effects induced by strain and curvature [3]. Thus, a methodology based on species diffusion adaptation to recover the flame response to low stretch rates, previously validated on spherical and counter-flow laminar configurations, is here challenged in turbulent cases [4]. Sub-grid flame-turbulence interaction models from the literature are assessed for their applicability to a lean H2/air mixture [5,6]. The impact of diffusion adaptation for thickened stretched flames is evaluated on a spark-ignition configuration with homogeneous turbulence using the TFM-AMR-Ignition approach [7].

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[7] E.Sandoval et al. doi:10.1016/j.combustflame.2022.112507

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CFD investigations of the ignition and stabilization processes of bluff-body lean premixed hydrogen flames

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Ignition and altitude relight are critical aspects in the design of a new aero-engine combustor, in relation to safety, reliability and operability. The utilization of hydrogen as fuel offers several advantages in terms of combustion performance and environmental impact although it is essential to consider the potential tendency to develop undesirable flame-holding locations and flashback scenarios. These phenomena are related to the higher reactivity of hydrogen and consequently to the major overpressure that arises during the ignition phase with respect to conventional jet fuels. Therefore, it is mandatory that the current numerical models can accurately predict transient processes as ignition and flashback. In this context, the atmospheric test rig installed at the Norwegian University of Science and Technology (NTNU) operating with a lean, perfectly premixed, hydrogen-air flame that stabilizes on a conical bluff body is considered. The complete hydrogen ignition sequence from spark release to full flame development (second phase) is numerically investigated with the pressure based ANSYS Fluent in the high-fidelity Large Eddy Simulations framework. The Thickened Flame Model coupled with an Energy Deposition strategy permits an accurate prediction of the most significant phenomena involved, validating the employed numerical strategy. Multiple operating conditions are explored, according to the experimental setup, allowing to investigate different ignition dynamics.

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Track04 Turbulent combustion

Track04-1 Turbulent combustion (1)

Chair: TBD
Wednesday, May 8; 10:40 - 12:20; Room A

Direct numerical simulation of a supersonic turbulent boundary layer with hydrogen combustion

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In the aim to guarantee reliable ignition and maintain sustainable combustion within supersonic combustors, a variety of injection strategies are employed including injections via steps, cavities, structures, and throttles. The interaction of flames with the intense shear found in near-wall turbulent flows is a common feature of these implementations. The goal of the present study is to comprehend the intricate mechanisms of turbulent flow in boundary-layer combustion, through the use of direct numerical simulations. The selected flow model is a non-premixed hydrogen-air flame, ignited within a three-dimensional supersonic turbulent flat-plate boundary layer, which operates at a Mach number of 2.44 and a friction Reynolds number of approximately 1000. The simulation involves a finite-rate model encompassing 9 species and 19 chemical reactions. The inlet flow consists of preheated air in the mainstream and a hydrogen film injected in proximity to the cold wall, inducing turbulent mixing via the Kelvin-Helmholtz instability and auto-ignition of the flame within the boundary layer. Classical statistical metrics for turbulent closures are assessed. It is found that the turbulent Prandtl number and the turbulent Schmidt numbers for each species tend to unity in the buffer layer but deviate from unity near the flame front. A spectrum analysis reveals that the strong Reynolds analogy is not satisfied near the flame front region due to a scale separation between velocity and temperature fluctuations. A statistical analysis of elementary reactions at different distances from the wall is provided, highlighting the dominance of hydrogen atom depletion in the near-wall heat release and the prevalence of water vapor production in the contribution of heat release near the boundary layer's edge.

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DNS of hydrogen flame stabilization in multiple jets in cross flow

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Pure hydrogen combustion in gas turbines (GTs) is extremely challenging due to its unique thermochemical properties, such as high diffusivity which can lead to flashback, and potentially high combustion temperature, which leads to NOx formation. "Micromix" combustion technology is a new approach that aims to address these challenges: by injecting hydrogen through an array of miniaturized jets, it has the potential to produce reliable and safe combustion while minimizing NOx formation. Development of this approach requires a detailed understanding of flame stabilization mechanism in the multiple jets in cross flow configuration. In the present work, a direct numerical simulation (DNS) of two non-autoignitive hydrogen jets issued into an air crossflow is reported. It is found that the flame along the jet centreline plane features two branches, one stabilized on the leeward side and one lifted above the jet trajectory. The windward reaction zone is thinner in the near field than the leeward one, while the lee-stabilized branch is found to be more stable due to the larger and stronger recirculation zones created downstream of the injection point. The results demonstrate that the flame stabilization is significantly affected by the interaction between jets, boundary layer, and the differential diffusion of hydrogen.

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Direct numerical simulations of head-on quenching of statistically planar turbulent premixed flames on flat and rough walls

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Rough walls are common in engineering applications. However, existing understanding of combustion near rough walls is lacking. In the present work, direct numerical simulations (DNS) of head-on quenching of statistically planar turbulent premixed flames on flat and rough walls are reported for the first time. Hydrogen is considered as the fuel because of its high importance in a zero-carbon economy. The wall heat flux and flame quenching distance statistics for laminar and turbulent premixed flames head-on quenching on isothermal inert walls with varying roughness are compared. The alignment quantity measured the angle between the flame normal vector at the quenching edge and wall normal vector on various rough walls are examined. The near-wall behaviors of intermediate species and reactions in head-on quenching are demonstrated. Finally, the model performances in the context of the flame surface density (FSD) and scalar dissipation rate (SDR) based reaction rate closures on flat and rough walls are explored.

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Direct Numerical Simulation of turbulent premixed combustion in a model turbulent flow with mean shear at Reλ = 140 and single reactive scalar Zeldovich rate closure

Aditya Vinod, Tejas Kulkarni, Fabrizio Bisetti
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Direct Numerical Simulations (DNS) of turbulent premixed flames are employed to study the evolution of the flame surface in the turbulent swirling von Kármán flow, which is characterized by intense shear-driven turbulence. The combustion closure features a single passive reactive scalar with a source term equal to the Zeldovich rate functional. Such a single scalar combustion model coupled with DNS of reactive turbulence is computationally affordable, enabling parametric studies at scale. Turbulent flames are initialized as a spherical kernel of burnt gases in the center of the device, where turbulent transport by velocity fluctuations is dominant, and propagate outwards. The Reynolds number is increased up to Reλ = 140 across three configurations holding the Damköhler number constant. The flame Surface Density Function is shown to scale in time according to a common function and found to be self-similar with respect to a similarity distance variable. The peak of the SDF is scaled by a power law of the Reynolds number with exponent nearly identical to that reported in recent numerical and experiment studies of turbulent spherically expanding flames. The form of the scaled and self-similar SDF explains the trends of flame area with increasing Reynolds number.

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On the occurrence of negative propagation speeds and negative divergence in turbulent premixed flames

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Based on the analysis of data from Direct Numerical Simulation of turbulent premixed flames with finite rate chemistry, we find that the propagation speed of reactive fronts in turbulent premixed flames takes instantaneous values that are negative in sign and large in absolute value. The ensuing probability density function of the propagation speed is complex: the PDF has a positive mean, is at times bimodal with two local maxima – one at positive and one at negative values for sufficiently high values of the Reynolds number, is skew-positive, and has a large kurtosis indicating extreme events. Further, negative displacement speeds correlate strongly with negative values of the velocity divergence and large values of the most compressive strain eigenvalue. We also find a clear dependence of the statistics of the rate of strain tensor on the Karlovitz number, whereby as the Karlovitz number decreases, the probability that all strain eigenvalues are positive increases for small values of strain. These results are fundamentally inconsistent with existing theory that explains changes to propagation speed with the effect of stretch. Instead, statistics appear to be closely related to classical mechanisms of scalar mixing in isothermal turbulence with Reynolds number effects pertaining to small-scale intermittency.

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Track04-2 Turbulent combustion (2)

Chair: TBD
Wednesday, May 8; 10:40 - 12:40; Room B

Relationship between Radial Pressure Gradient and Flame Macrostructure in NH3/H2/Air Premixed Swirl Burners

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This work investigated the influence of radial pressure gradient on flame macrostructure in NH3/H2/Air fueled premixed swirl burners operating in rich-lean staged combustion. Five different burner geometries were operated at equivalence ratios from 0.72 to 1.10, hydrogen mole fractions from 0% to 27%, and jet Reynolds Numbers from 500 to 21,000. Type I, II, III and IV flame macrostructures were identified using OH* and NH2* chemiluminescence. Measured radial pressure gradient of the fuel-air vortices was compared against theoretical radial pressure gradients of free and forced vortices. The measured pressure gradient for type I and II macrostructures corresponds to a pressure gradient typical of free vortices while the measured pressure gradient for type III and IV macrostructures corresponds to that of a forced vortex. Characterizing the radial pressure gradient and flame macrostructure provides a basis for validating LES and DNS simulations. Understanding the influence of burner operation on flame macrostructure allows for design of burners with smaller computational domains, reducing simulation cost. Finally, the fueling and emissions associated with rich and lean combustion zones of the swirl burner were investigated to provide boundary conditions for simulating the lean burn zone as a laminar diffusion flame, further reducing computational cost.

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Local Curvature and Speed of Turbulent Premixed Ammonia and Blends with Methane and Hydrogen Flames in a Spherically Expanding Configuration

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Ammonia (NH3) appears a promising zero-carbon fuel, however most energy conversion systems require a combustion promoter such as Hydrogen (H2) or Methane (CH4) to guarantee start-up, stability and combustion efficiency. Yet, there remains limited studies for ammonia combustion under relevant turbulent conditions. To that end, the outwardly propagating flame configuration was employed to determine turbulent propagation characteristics of various ammonia blends, employing Mie-Scattering tomography coupled with numerical analysis facilitating flame structure investigation. Three Ammonia based blends were selected (60%NH3 – 40%H2 φ = 0.8, 70%NH3 – 30%H2 φ = 1.0, 40%NH3 – 60%CH4 φ = 1.0), exhibiting ostensibly similar laminar burning velocities (SL0) but different flame stretch sensitivities (Lewis Number (Le), Markstein Length (Lb)); allowing to gain insight on the effect of flame stretch and wrinkling effect at constant turbulent intensity to laminar flame speed ratio (u'/SL0) and ratio of integral length scale and flame thickness (LT/δG). Enhancement in turbulent flame speed was observed to increase with decreasing Lewis number and Markstein Length. This observation was supported by local flame analysis. With a decrease in Le and Markstein Length, the probability density function (PDF) of curvature at a fixed eddy turn over time distinctively spread towards greater negative curvatures coupled with the appearance of high-speed values on the negative curvature side. Furthermore, an increase in the stretch factor (I0) was observed with blends containing highest amount of H2, opposite to the trend in wrinkling ratio. These results in turbulent NH3-based flame behaviour are thought to invariably impact practical combustion systems.

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Combustion characteristics of NH3/O2 pintle engines

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Combustion characteristics of oxidant-centered NH3/O2 pintle engines under different total momentum ratio conditions and different mixing ratio conditions are studied by a two-dimensional numerical simulation using a detailed 80-step chemical reaction mechanism of ammonia. Results show that high chamber pressure can achieve high combustion efficiency at a mixing ratio of 1.2. The high chamber pressure can promote the mixing and combustion of the fuel and oxidizer, increasing the combustion rate, which can release the energy of the fuel more quickly, improving the combustion efficiency. A mixing ratio of 0.96 and a total momentum ratio of 0.93 have a high combustion efficiency at a chamber pressure of 4.8 MPa. When the mass flow rate of oxygen is close to the mass flow rate of ammonia, this means it is at a stoichio-

metric ratio, and when the total momentum ratio is close to unity, it can enhance the mixing, further strengthening the complete reaction, and thus, improving combustion efficiency.

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INVESTIGATION OF AMMONIA (NH3) COMBUSTION WITH DIESEL PILOT IGNITION

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All transportation sectors are seeking methods to decarbonize their energy sources. For high energy consumption applications (e.g. large marine, locomotives), ammonia is a potentially attractive carbon-free fuel option, primarily due to its ~2x volume energy density compared to very high pressure gaseous hydrogen. With a desire to retain full diesel capability, one approach to use ammonia as a fuel is a dual fuel concept where ammonia is pre-mixed with air and then ignited by the diesel injection.

This paper considers the mechanisms of ammonia-diesel dual-fuel combustion. The dual fuel combustion process is complex, relying on the injected diesel fuel to ignite and combust the ammonia and air mixture. The ammonia-diesel, dual-fuel combustion is a mixture of diffusion burning, in the case of the diesel pilot, and of flame propagation, in the case of the ammonia not entrained in the diesel jet. The combustion computational fluid dynamics (CFD) simulation provides insight into the understanding of ammonia-diesel dual-fuel combustion, including limitations on ammonia substitution and methods for reducing ammonia emissions. An ammonia combustion kinetic mechanism was identified in the literature and merged with the diesel kinetic mechanism to form a dual-fuel mechanism for the simulation. The model was refined to better match the experimental data for the laminar flame speed of ammonia versus equivalence ratio published in the literature. The simulations identified multiple mechanisms critical to diesel-ammonia dual fuel combustion. The dominant mechanism is dependent on the ratio of ammonia to diesel, the substitution ratio (SR), and the air-ammonia equivalence ratio.

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Large-eddy simulations of hydrogen-enriched natural gas flames in a trapped vortex combustor

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The trapped vortex combustor (TVC) is a promising technology for premixed combustion with fuel flexibility. This combustion configuration promotes better fuel-air mixing and has the potential to reduce emissions. Depending on the flow configuration, a TVC can operate in rich burn, quick quench, and lean burn (RQL) mode which is investigated in the present study. Particularly, we employ high-fidelity large-eddy simulations (LES) to investigate the flame stabilization mechanism and flow-chemistry interactions. The TVC configuration comprises a channel that expands into a unity aspect-ratio cavity, which locks the primary vortex and stabilizes the flame. While a lean premixed mixture is introduced at the inlet of the channel, a rich mixture is injected at the bottom of the cavity. The simulations were conducted using OpenFOAM, an open-source C++ library for computational fluid dynamics (CFD). The k-equation subgrid model and the partially stirred reactor (PaSR) model were implemented for the closure of sub-grid scale terms. To investigate the effect of the addition of hydrogen, we considered two cases: one with pure methane and the other with a 50-50 mixture of hydrogen and methane. The overall equivalence ratio is kept constant at 0.7. The results from the simulations are compared with experimental OH planar laser-induced fluorescence (PLIF) data. It is observed that the addition of hydrogen inhibits the unsteadiness in the combustion process and improves the penetration of the cavity flow into the main channel flow, which in turn enhances the pattern factor. A quantitative assessment of these aspects will be presented.

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Large Eddy Simulation of Flame Flashback Phenomenon in a Model Scramjet Combustor Utilizing a Strut-Cavity Flame Holder

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Efficient hypersonic air-breathing propulsion, crucial for cost-effective payload launches, faces challenges such as inadequate combustion due to short flow residence times. The development of efficient scramjets relies on flame stability. Despite the widely held belief that acous-

tic disturbances cannot propagate in supersonic flowfields, evidence shows instances of flame flashback. Existing scramjet studies on flashback lack consensus, necessitating thorough research. Supersonic turbulent combustion simulations, conducted with the OpenFOAM solver within a large eddy simulations framework, involved three-dimensional, transient, and multi-species chemically reacting conditions. We explored a novel strut-cavity flame holder configuration, confirming simulation accuracy against DLR's strut design data. Flame lift-off was observed in the base case with a strut configuration akin to previous findings. A 9-species, 27-reaction Arrhenius model investigated hydrogen fuel flame behaviour during flashback scenarios. RANS simulations fine-tuned flame holder design parameters. The shear layer, originating from the cavity corner's leading edge, impinges on the transverse fuel injection from the rearward step of the offset cavity. This impingement results in a complex flow field around the strut-cavity flame holder, characterized by interactions between shear-layer shock phenomenon, cavity recirculation zones, and the trajectories of both the shear layer and fuel. LES directly influences fuel and oxidizer mixing, impacting chemical reaction rates and combustion efficiency. LES effectively depicts turbulent flame dynamics, examining flame structures and their interactions with shocks and the turbulent flow field. This study aims to understand the intricacies of combustion and the factors contributing to supersonic flame flashback using large eddy simulation.

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Track04-3 Turbulent combustion (3)

Chair: Shinji Nakaya
Wednesday, May 8; 13:30 - 15:10; Room A

Study of turbulence back-scatter in a laboratory-scale swirl stabilized aero-combustor using DNS

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Classical theories of turbulence suggest that the kinetic energy cascade in nonreacting flows has a net transfer of energy from large to small scales. However, previous studies demonstrated that the thermal expansion of premixed flames can reverse the flux of energy through the injection of energy at flame scales into larger scales, resulting in back-scatter. These observations were confirmed experimentally for a premixed laboratory-scale aero-combustor. However, it is unknown whether backscatter also occurs in partially-premixed combustion in a swirl-stabilized combustor undergoing localized extinction/reignition near the lean blowoff limit. In this limit, edge flame propagation is found to exist, and it's structure presents a premixed leading edge that generates large thermal expansion compared to non-premixed flames, acting as a source of flame-generated backscatter. Direct numerical simulation (DNS) of a laboratory-scale swirl stabilized aero-combustor is performed for a reacting Jet-A liquid spray flame and backscatter is quantified from the filtered and subgrid kinetic energy transport equations evaluated in physical coordinates. It is found that edge flames lead to an inversion of the turbulent kinetic energy cascade at scales close to the flame thermal thickness. The back-scatter occurs within the flame brush and correlates with dilatation generated by thermal expansion. The total pressure gradient-velocity correlation term is also observed to produce kinetic energy at subgrid scales due to subgrid fluctuations in the pressure field caused by turbulent combustion. Hence, aero-combustors undergoing blow-off are more prone to back-scatter due to the development of edge flames that propagate to reignite previously extinguished regions.

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A study of the relation among flame surface geometry, flow and heat on premixed turbulent flames using DNS

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The surface geometry of premixed turbulent flame interacts with flow and heat. This study focuses on the relation among the flame surface geometry based upon flame curvature, local flow and heat on premixed turbulent flames using DNS (Direct numerical simulation). This analysis is performed by using DNS data of premixed turbulent flames (Nishiki et al., CTM 10 (2006), Tsuboi et al., JTST 3 (2008)). The flame surface geometry is considered by mean flame curvature and Gauss curvature on the prescribed iso-surface of the reaction progress variable defined by temperature. The flame surface geometry based upon the aforementioned curvatures varies with the reaction progress variable even though the premixed turbulent flames on the DNS data is located near the boundary between the wrinkled flamelets regime and the corrugated flamelets regime on the diagram of premixed turbulent combustion. This study makes a detailed analysis of the relation among the flame curvatures, local flow and heat with the different iso-surfaces of the reaction progress variable.

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DNS of multi-stage ignition in a simplified gas turbine premixer

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With the increasing need for fuel-flexibility, mitigation of auto-ignition inside gas turbine (GT) premixers has become crucial. GT premixers must be designed to ensure sufficient fuel-air mixing while avoiding the potential occurrence of auto-ignition, a challenge that requires a detailed understanding of turbulent mixing and chemistry interaction. Here, direct numerical simulations of a downscaled and simplified version of a GT premixer are presented. The configuration consists of multiple hot air jets in a fuel-rich crossflow (Rej=4000) at high pressure. A fuel blend of methane and dimethyl ether (DME) is chosen with a recent reduced chemical kinetics model validated in GT conditions. The addition of DME drastically increases the explosivity of the fuel mixture and causes a multi-stage ignition to occur, each stage resulting in a corresponding flame. For each stage we track the temporal evolution of individual ignition kernels in both physical- and phase-space, and assess their propagation mode through chemical explosive mode analysis. The observed ignition events differ for the different stages, with large ignition patches for low temperature ignition and quickly growing small kernels for high temperature ignition. In all cases, both diffusion and auto-ignition contribute significantly to the subsequent flame stabilization.

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Direct Numerical Simulation of Low-Emission Staged Ammonia Combustion

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Ammonia is a potential carbon-free alternative to natural gas in dispatchable power generation. However, burning ammonia in typical lean premixed gas turbine combustors leads to high levels of nitrogen oxide emissions. A promising strategy to mitigate such emissions is the staged rich-quench-lean (RQL) approach. With the RQL approach, an ammonia fuel-rich flame is stabilized in the primary combustion zone (PCZ), where fuel-bound nitrogen is converted in an oxygen-depleted environment, minimizing nitrogen oxide emissions. A secondary combustion zone (SCZ) comprises injection of air leading to the consumption of hydrogen that is present in the products from the PCZ. We present Direct Numerical Simulation (DNS) of a simplified SCZ configuration, namely transverse injection of cold dilution air into a cross-flow of hot hydrogen-containing pyrolyzed ammonia combustion products at equilibrium, at thermochemical conditions comparable to those of a heavy duty stationary turbine. The DNS shed light on the turbulent combustion and flame stabilization process of the SCZ, as well as emission formation in the SCZ and further downstream of the air injection. Three cross-flow equivalence ratios (1.1, 1.2 and 1.3) are simulated to study the impact of different air split ratios. An additional DNS is presented where a small amount of ammonia slip is present in the boundary regions of the flow, illustrating the detrimental effect ammonia slip can have on the performance of the RQL strategy.

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A DNS study of ignition characteristics of NH3/H2/air mixtures under RCCI marine engine conditions with hydrogen injection strategy

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Ammonia (NH3) is gaining interest as a carbon-neutral alternative in transportation applications, especially in the maritime sector. Nevertheless, using NH3 as the primary fuel for engines encounters challenges due to its low reactivity and flame speed. Hydrogen (H2) emerges as a promising additive to address the reluctance to combust of NH3. Two-dimensional direct numerical simulations (DNS) are employed to elucidate the effects of H2 injection on the ignition characteristics of NH3/H2/air mixtures under medium-speed marine engine conditions. NH3 is injected as port fuel, with an initial H2 injection occurring early to enhance the reactivity of NH3 and a subsequent H2 injection near the top dead center (TDC) to induce reactivity stratification. A compression heating model is incorporated into the DNSs to simulate the rise in pressure resulting from the piston motion. Accounting for the cooling effect attributed to the second H2 injection, a pseudo H2 species is introduced. Chemical Explosive Mode Analysis (CEMA) investigates the intricate interaction among reactivity stratification, cooling effects, and turbulence intensity. Comparative analysis with a single H2 injection reveals that the split injection strategy can defer early ignition by generating stratified combustion. Conversely, the split injection strategy accelerates the ignition process for late ignition scenarios.

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Track04-4 Turbulent combustion (4)

Chair: Andreas Kempf
Thursday, May 9; 09:50 - 12:30; Room A

Physics-constrained neural-network sub-grid-scale model for a flame in isotropic turbulence

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A neural-network sub-grid-scale model for large-eddy simulation (LES) of turbulent reacting flows is developed. A key aspect is that the closure model is trained a posteriori—on a model-predicted observable. This is more robust than the a priori approach, where the objective function would be based on the model itself. Our approach requires the end-to-end sensitivity of the observable with respect to the parameters of the model, which is computed using a discrete-exact adjoint solver. It is demonstrated on a statistically planar premixed flame in isotropic turbulence with one-step single-species irreversible chemistry in a thin-reaction-zone regime. The model is constrained to preserve Galilean invariance and local conservation, and also not to introduce spurious oscillations in scalar fields. We first train the model so its short-time prediction on the instantaneous field matches that of a direct numerical simulation. The trained model is then applied for a longer-time LES. Finally, the model is evaluated in terms of turbulent energy spectra and the turbulent flame speed.

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Filtered turbulent flame model: numerical principle and performance

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Modelling the interaction between flame and turbulence under the resolved scale depends on the closure reasonability. Physically, the flamelet assumptions remain reasonable in typical combustion simulations. Therefore species mass fractions and temperature can be mapped onto the mixture fraction, scalar dissipation and other relevant quantities. However, critical modeling closure problems do exist, especially the assumed joint probability density functions (PDFs) to calculate the filtered or mean field quantities. Aiming for such challenge issues, a newly proposed filtered turbulent flame model is implemented in the framework of large eddy simulations for non-premixed turbulent combustion. The general principles of model realization are developed, including the structure and physics of the filtered flame, tabulation setup, and the numerical algorithm. Because of the involved modeling parameters for tabulation can be directly calculated from either the resolved or subgrid model quantities, the filtered turbulent flame model is in principle favorable to improve the numerical predictability. Tentative numerical tests and comparisons with other models justify this modeling idea. Possibilities for further improvements and the numerical principles are also addressed.

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Direct moment closure model coupled with acceleration algorithm for LES of turbulent partially premixed dimethyl ether jet flame

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The development of a turbulent combustion model for partially premixed flames remains a significant challenge due to the coexistence of premixed and non-premixed modes. In this study, the Direct Moment Closure (DMC) model, known for its methodological applicability to various combustion regimes, has been extended to multi-reactant reactions with closure of higher-order moments. The DMC model has been applied to simulate a benchmark flame of a piloted partially premixed dimethyl ether jet flame in the TNF Workshop. The Large Eddy Simulation with DMC model (LES-DMC) results have been compared with experimental data and results from the literature. Remarkably, the DMC model exhibits excellent performance in predicting the spatial distribution and mixture fraction-conditional average of velocity, temperature, mixture fraction, and mole fraction of major and minor species. The accuracy and efficiency of the acceleration algorithms, coupled with LES-DMC, have been thoroughly assessed. As a result, the overall computational cost of LES-DMC-TDAC is significantly reduced to 45%. The simulation results have facilitated a detailed analysis of the characteristics of the partially premixed dimethyl ether flame.

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On Flamelet calculation methods to incorporate effect of flow strain in presence of large heat loss in turbulent flame propagation models

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Incorporating effects of heat loss and flow strain on the turbulent flame propagation is of wide interest for capturing flame shape and instabilities in practical combustion chambers. For lean-premixed combustion systems, a canonical laminar counterflow premixed flame is used to tabulate the laminar flame speed variation with varying strain rate and heat loss through enthalpy defect - chemical or sensible. The laminar flame speed becomes a factor in turbulent flame propagation speed models, thereby incorporating heat loss and strain effects in actual flame propagation. However, correlation of strain rate (local or global) obtained from the canonical flames with that obtained for turbulent flows in combustion chamber using CFD (mostly Large Eddy Simulations) is somewhat qualitative. Also, large heat losses necessarily require use of chemical enthalpy defect, which can interfere with some assumptions needed to capture the strain rate effect, such as using 'fresh against burnt' counterflow setup and not the 'reactant against reactant' or the 'twin flame'. Such details are not immediately obvious to practicing CFD engineers and may lead to erroneous modelling. This presentation discusses details of calculation methods of canonical laminar flames to capture the effect of strain in presence of high heat loss for a practical turbulent flame. Results are presented in terms of flame stabilization near walls with large heat loss for a tangential inlet swirl premixed burner case from literature and compared with experimental data to highlight modelling recommendations.

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DEVELOPMENT OF A VIRTUAL CHEMISTRY REACTION MECHANISM FOR H2/CH4 TURBULENT COMBUSTION MODELLING

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The species transport models are one of the most attractive solutions to capture complex phenomena such as differential diffusion stretch and heat loss on the flame front. One of the biggest drawbacks of these combustion models is the high computational cost that can become prohibitive when higher-order hydrocarbons have to be included in the fuel mixture. The need to reduce the number of species to be transported and the complexity of the reaction mechanism raises the need to develop "ultralight" kinetics schemes.

In this work, a virtual reaction mechanism has been proposed and derived for the investigation of H2/CH4 combustion. Since the differential diffusion is expected to play a pivotal role in high H2 content mixtures in lean conditions, the proposed model accounts for the differential diffusion of the fictitious species. The predictivity of the virtual chemistry model has been validated on a turbulent combustion test case at atmospheric pressure. In the LES simulations, the Thickened Flame Model has been adopted for modelling the turbulence chemistry interaction. The numerical results are compared with OH* chemiluminescence measurements to assess the prediction capability of the virtual chemistry reaction model in reproducing the flame shape detected in the experimental campaign.

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Numerical Modelling of Local Extinction in Sydney Swirling Non-Premixed Flames using LES/FGM

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Flame extinction emerges as a fundamental exploration within combustion theory and contemporary combustor design for gas turbines, particularly near lean blowout. Employing Large Eddy Simulation (LES) and Flamelet Generated Manifold (FGM) methods, the study simulates the Sydney swirl-stabilized non-premixed methane flames, exhibiting varying degrees of local extinction. The FGM framework demarcates chemistry through mixture fraction and reaction progress, constructing the manifold via 1D counter flow flamelets. Examining statistics encompassing velocity, mixture fraction, and major species mass fractions in physical and mixture fraction space reveals good alignment with experimental measurements. The level of local extinction with increased fuel bulk velocity velocities is reasonably captured, revealing its manifestation through a very low heat release rate, reduced OH mass fraction and temperature, and relatively high scalar dissipation. In contrast to conventional indicators, the findings emphasize the significance of considering multiple factors to identify local extinction events accurately.

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Clipping-free fine structure's mass fraction region for low turbulence Eddy Dissipation Concept model

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To predict strong turbulence-chemistry interactions as in Moderate or Intense Low oxygen Dilution (MILD) combustion regime, the Eddy Dissipation Concept (EDC) model has been successfully applied using Reynolds- Averaged Navier-Stokes (RANS) or Large-Eddy Simulations (LES) modeling. However, several studies of the Jet in Hot Co-flow (JHC) configurations have shown that in its standard formulation it overpredicts the maximum temperature level in MILD regimes, due to overestimated overall reaction rate. It is assumed that the reactions take place in the regions of the flow where the dissipation of turbulence kinetic energy takes place. The mass fraction of the fine structures $\gamma\lambda$ is provided by an energy cascade model. In various numerical codes, an upper limit for $\gamma\lambda$ is 0.7 - 0.9 for low Reynolds (Re) numbers. To avoid misunderstanding and trivial $\gamma\lambda$ limit, and based on the Direct Numerical Simulations (DNS) normalized reaction rate values comparison, three formulations (velocity- and length scale-based) were selected and validated, using Ansys Fluent, against the Delft JHC burner (low turbu- lence), and Sandia Flame C and D (high turbulence), to ensure alignment with the developed original EDC model assuming high turbulence. The results show a reduction in temperature peaks by implementing new revised pos- tulates. In the case of Sandia D, two low turbulence postulates lead to the flame extinction (unscaled); for Sandia C only one, as expected, due to low $\gamma\lambda$ values at low Re. They exhibit similar performance to the original EDC downstream of the flame, with some underpredictions near the burner nozzle, when scaled (to converge with the original EDC at high Re) or blended for a moderate turbulence transition zone and the original EDC formulation for high Re (shrinking cascade model: 1-, 2-, or 3-level energy cascade). The research is ongoing, and we look forward to sharing our finalized results and insights during the conference involving variable reacting fraction χ implementation, results with additional Re blending limits (to achieve broader spectrum of Re), and eventually run a priori DNS test of the hybrid (blended) model.

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Effects of cryogenic temperature on turbulent premixed hydrogen/air flames

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As a carbon-free fuel, hydrogen (H2) is of increasing importance in the development of low-emission engines. Due to a low volumetric energy density, H2 is preferably stored at cryogenic temperatures (Tu≤100 K). In this context, it is indispensable to investigate the combustion behavior of hydrogen at such low temperatures. Although some studies focused on the ignition and detonation of hydrogen, investigations about premixed H2/air flame propagation interacting with turbulence at cryogenic temperatures are rather scarce. In this work, stoichiometric turbulent premixed H2/air flames are studied at cryogenic temperature (Tu=100 K) and normal temperature (Tu=300 K), using three-dimensional direct numerical simulations with detailed chemistry and transport. It is found that at cryogenic temperature, dimensionless turbulent flame speed and flame surface area increase significantly due to Darrieus-Landau instability (DLI) induced by a large expansion ratio. Since the effective Lewis numbers of the two cases are close to unity, the diffusive-thermal instability (DTI) is negligible in the cases. Furthermore, it is found that there are substantial differences in the peaks of HO2 and H2O2 mass fractions between the two cases, probably due to smaller local flame curvatures at cryogenic temperature. Moreover, the results indicate that the flame response to stretch is not sensitive to the change of the initial temperature. A larger fractal inner cutoff scale is found at Tu=100 K, suggesting that the flame exhibits more large-scale flame wrinkling than that at Tu=300 K due to the impact of DLI. All these facts lead to the conclusion that cryogenic temperature can significantly promote large-scale flame wrinkling, increase turbulent flame speed and flame surface area, and affect intermediate species distribution. This suggests that combustion of cryogenic H2 may have a high risk of flashback.

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Track04-5 Turbulent combustion (5)

Chair: Benoît Fiorina
Friday, May 10; 09:50 - 12:10; Room A

Experimental and Numerical Investigation of Lean Blowoff Dynamics in Swirl-Stabilized Premixed Flame

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Lean premixed combustion (LPC) holds great potential for reducing NOx emissions; however, it poses the challenge of increased blowoff risk. This study comprehensively investigates swirl lean-premixed n-butane/air flames, focusing on the differences between stable flames and those nearing blowoff. Experiments employing Particle Image Velocimetry (PIV) were conducted to analyze flow fields, while Detached Eddy Simulation (DES) modelling, incorporating the Flamelet Generated Manifold (FGM) model and USC-Mech reduced chemical mechanism, provided further insights. The results reveal notable distinctions in the near blowoff flames, including a lower high-temperature zone, enhanced heat loss due to flame-vortex interaction-induced low-temperature spots, higher strain rates, and turbulence fluctuations influencing flame attachment, and the emergence of a Processing Vortex Core (PVC) downstream. These findings highlight the combined influence of fuel/air mixture ignition, PVC instability, and flame attachment lift-off in lean blowoff occurrence. Understanding these mechanisms is vital for developing effective strategies to prevent or manage lean blowoff, ensuring efficient and low-emission LPC systems.

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Performance of flame surface density and scalar dissipation rate based mean reaction rate closures for fuel-lean hydrogen-air turbulent premixed flames

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Hydrogen is often identified as one of the future fuels to meet net-zero targets. However, the validity of conventional mean reaction rate closures, which were benchmarked for hydrocarbon-air flames with Lewis numbers close to unity, is yet to be assessed for lean H2-air premixed flames. In the present work, mean reaction rate closures based on flame surface density (FSD) and scalar dissipation rate (SDR) have been assessed based on three-dimensional direct numerical simulations (DNS) of statistically planar turbulent premixed hydrogen-air flames at equivalence ratios of φ = 0.4 and 0.7 under different turbulence intensities. It has been found that mixture fraction dependence of the reaction progress variable has a significant influence on the performances of FSD and SDR closures and this effect is particularly strong for φ = 0.4. The stronger preferential diffusion effects at smaller equivalence ratios negatively affect the FSD closure predictions, whereas the SDR closure is relatively less sensitive to the variations of equivalence ratio.

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Dynamic Tracking of Surface Topology in Turbulent Premixed Flames using Machine-Learning

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In turbulent premixed flames, the topological evolution of the local flame surface can alter the balance between flame area generation and destruction which in turn has a profound influence on global flame propagation. In this work, local annihilation of flame area resulting from flame-flame interaction is used to classify the corresponding interaction topology obtained from a DNS dataset of a methane-air turbulent premixed flame. Principal flame configurations are identified as reactant pocket, product pocket, tunnel closure and tunnel formation. A machine-learning classification algorithm is then trained to map the previous point-based classification to local surface interaction. With this method, local changes in the flame surface that alter flame speed may be tracked dynamically. The classification accuracy for complex real-world interaction is 77% - while for clean isolated interaction events, the accuracy is near-perfect. Moreover, the algorithm is shown to recognise key topological features of each principal configuration and works well for a range of turbulent intensities. The main advantage of this method is the potential for incorporating and subsequently tracking additional flow properties such as turbulent straining and local displacement speed. The aim is to develop more robust burning and stretch rate models.

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Role of Dilatation in the Injection and Redistribution of Turbulent Kinetic Energy in Premixed Reacting Flows

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The nature of the flame effects on the surrounding turbulent flow is one of the central open questions in turbulent combustion, as the flame can fundamentally alter the dynamics of the turbulent cascade. In our prior work, we have shown the ability of a flame to generate significant turbulent intensities on scales much larger than the characteristic flame width even in the absence of external turbulent energy injection. Such flame-generated turbulence was observed in compressible regimes through the action of a baroclinic torque. Here we present the first numerical evidence of pronounced turbulence generation by the flame in low-speed regimes not by baroclinic torque, but rather through flame-induced dilatation. We first characterize the properties of such turbulence by analyzing data from DNS. The wavenumber scaling of the dilatation spectrum is shown to be linked to the fractal dimension of the flame front. This relation is then used to obtain the spectrum of the kinetic energy injection rate, which is then used to explain the observed kinetic energy spectra of the flame-generated turbulence. The dependence of the strength of turbulence generation on the flame density ratio is also examined. Finally, we discuss the implications of these results for turbulent combustion modeling.

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On flame displacement speed variation due to flame-flame interaction

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Enhancement in the local flame displacement speed due to flame-flame interaction has been reported in the literature. Recently, models capturing this enhancement as a function of parameters pertaining to the local flame structure have been developed. However, these models have been validated for statistically planar flames in isotropic turbulence. Additionally, local turbulent straining and flame broadening strongly affects local flame displacement speed at zero local curvature, depending on effective Lewis and Karlovitz numbers. Considering that the local flame displacement speed is a manifestation of the local statistics, a fundamental question arises: to what extent do the configuration and additional complexities like shear flows govern the density-weighted local flame displacement speed? To address this question, the current study investigates two DNS cases of freely propagating turbulent lean premixed hydrogen-air flames in a box configuration at Lewis numbers 0.5 and 1, and a third DNS case of turbulent methane-air jet flame at Lewis number 1. The local flame displacement speed was enhanced over its laminar value at large negative curvatures in all configurations. On average, the flame surfaces are thickened at the most probable regions (near zero curvature) compared to the strained laminar counterpart. The reasons and implications of thickening on density-weighted local flame displacement speed are explored.

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Differential diffusion modelling for LES of a hydrogen-fuelled swirled burner with axial air injection

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A swirled stabilized combustor with axial air injection (AAI) is analysed by means of large eddy simulation (LES) with flamelet combustion model and presumed filtered density function (FDF) closure. A case employing a fuel blend of 75% CH4 and 25% H2 in volume is simulated to gain insight on the reacting flow features and to validate the model against in house experimental data. The analysis is extended to H2 /air combustion at the same power setting to evaluate hydrogen effects on emissions and identify criticality in flame stabilization. Two approaches to include differential diffusion in the thermochemistry database and at the resolved scales are tested. Results reveal how fuel/oxidizer mixing plays a predominant role in flame stabilization, temperature and emissions. In particular, axial air injection is observed to noticeably affect the swirling flow field in the mixing tube and consequently the flame-burning conditions. The inclusion of differential diffusion modelling is observed to enhance mixing and modify the equivalence ratio distribution at the entrance of the combustion chamber. Additionally, local reaction rate variations on the flame, coupled with flame front curvature, are observed to influence the flame stabilization location, local temperature and NOx emissions.

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Large eddy simulation of a turbulent jet ignition process of hydrogen lean mixture with a super-rich pre-chamber

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A super-rich-burn, quick-mix, lean-burn (SRQL) combustion strategy for hydrogen internal combustion engines using active pre-chamber is proposed to achieve stable ignition under lean-burn conditions and mitigate nitrogen oxide emissions resulting from high combustion temperatures during hydrogen turbulent jet ignition (TJI), simultaneously. To investigate the ignition and quenching mechanisms in the strategy above, combustion behaviors of the super-rich transient turbulent jet ignition process in globally lean mixtures were simulated by Large Eddy Simulation (LES) using OpenFOAM. Dynamic sub-grid scale model and the Partially Stirred Reactor (PaSR) combustion model were integrated into the simulation. The calculated results for different nozzle diameters were analyzed and compared with the experimental results in a Rapid Compression Machine (RCM). Simulation results showed the reproducibility of the SQRL-TJI process in terms of the auto-ignition of the hot jet and the flame lift-off phenomena. Based on the simulation results, the mixing process of hot jets was investigated, and the local Damköhler numbers' behaviors over time were calculated quantitatively.

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Track04-6 Turbulent combustion (6)

Chair: Michael E Mueller
Friday, May 10; 13:00 - 15:00; Room A

Manifold-based modeling of supersonic turbulent combustion: Direct inclusion of high-speed effects

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Manifold-based models for turbulent combustion are usually derived in the low Mach number limit where pressure variation and viscous heating are assumed to be negligible. These low Mach approximations result in enthalpy becoming a conserved scalar that varies linearly with respect to mixture fraction. While approaches have been developed for high-speed combustion that ensure a consistent thermodynamic state between the flow solver and the combustion model, these approaches still rely on the low Mach number formulation of the manifold equations and do not consider the direct influence of high-speed effects on the enthalpy and its variation with mixture fraction. In this work, a truly high-speed manifold-based combustion model for nonpremixed combustion that directly incorporates high-speed effects is proposed. The model requires closure of the pressure variation and viscous heating terms, and an a priori study is performed using high-fidelity data from a high-speed turbulent reacting flow in a scramjet-like geometry to investigate these high-speed terms and their dependence on mixture fraction and other flow parameters.

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Numerical simulation of CH4/LOx supercritical flame

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The oxi-combustion of methane is studied by high-fidelity simulations in the context of liquid rocket engines. The pressure thus exceeds the critical pressure of incoming fluids but stays below the critical pressure of water. Methane and oxygen are injected at cryogenic temperatures in a splitter plate configuration that mimics a small part of a co-axial injector. Simulations are performed with a reduced chemistry containing 17 species and 44 reactions, along with a specific treatment for thermodynamics and transport properties to address real-gas effects. The resulting flame is stuck between two dense flows that locally modify the turbulent kinetic energy. Consequently, the flame can split and experience different regimes of combustion: non-premixed, lean, and rich premixed. Accordingly, species concentration varies with the flame regime and OH is only found in regions poor in methane, contrary to H2O. For the latter, depending on the local temperature, a part of it should be in liquid or even solid phase meaning that additional modeling effort should be performed in the future. Large-eddy simulations are also conducted using a no-model assumption or the TFLES approach for the subgrid species source term.

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Study on soot oxidation and leakage in a turbulent non-premixed jet flame

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Soot particle evolution in turbulent flames is complex and involves a wide range of timescales, including the slow soot-formation processes and fast consumption due to oxidation. Accurate modeling of the soot-chemistry-turbulence interactions is fundamental for the accurate prediction of soot emissions, but these interactions are still not fully understood. Direct Numerical Simulation (DNS) is a key tool for the development of more accurate predictive models. In this work, a new DNS of a three-dimensional temporally evolving turbulent non-premixed jet flame is presented. The chosen configuration is specifically designed to study the later stages of soot evolution, overcoming limitations seen in previous DNS studies of sooting flames. A particular focus on events of soot leakage in the lean side of the flame ("Soot breakthrough") due to incomplete soot oxidation processes is posed. A characterization of soot breakthrough and its correlation with the gas-phase quantities, such as mixture fraction and oxidation-relevant species, is provided. The presented DNS data is then compared with a previous DNS study with a similar configuration where strong oxidation, but negligible soot leakage, were obtained. Effects of finite-rate soot oxidation events on the evolution of soot particles are discussed, together with some implications for soot subfilter models in Large Eddy Simulations.

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Influence of Turbulence on Soot formation in Iso-octane Outwardly Propagating Rich Unstable Flames

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Soot formation in outwardly propagating iso-octane rich turbulent flames was investigated by means of two-dimensional numerical simulation at a mixture equivalence ratio of 1.4. The soot formation in the cusp area of the turbulent flames was larger compared to that in the area convex toward the unburned mixture. The soot inception and surface growth processes at the cusp area were enhanced by an increase in the concentration of C2H2.

The cusp area had a negative flame stretch rate; in contrast, the convex area had a positive flame stretch rate. Flame temperature in the negatively stretched cusp area decreased due to thermo-diffusive effects because the Lewis number of the rich iso-octane flames was less than unity. Larger C2H2 concentration and soot formation in the cusp area were found to be caused by the decrease in the flame temperature due to the negative flame stretch in this area.

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Numerical assessment for turbulent partially-premixed combustion using reaction-diffusion manifold based model reduction "on the fly"

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Partially-premixed combustion (PPC) often presents a challenge for model reduction methods, because an a priori identification of types of combustion is needed. Here, we use a generalized reaction-diffusion manifold (REDIM)-reduced chemistry approach to investigate such mixed-mode flames, which overcomes the drawback of the need of an a priori knowledge. To include the information about the combustion system, gradient estimates are provided during the generation of REDIM, simultaneous to the solution of the conservation equations. An iterative methodology is used in this work to provide the gradient estimates for REDIM generation. In this methodology, reduced calculations are coupled with the generation process of REDIM itself such that the manifold evolves automatically according to diffusion-related information provided by the combustion system. In this way, prior knowledge about the combustion system becomes minimal and no information is needed from a detailed system. Large eddy simulations for Sydney turbulent PPC with inhomogeneous inlets is performed using the dynamic thickened flame (DTF)-REDIM model. The good agreement between calculated and measured values for temperature, major and minor species mass fractions shows that the method can produce realistic reduced models also for systems with complex interactions of chemical reaction, molecular transport and flow, like turbulent PPC.

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Controlling the resolved flame thickness of diffusion flames in LES with filtered tabulated chemistry

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LES of turbulent non-premixed flames remains important for the design of novel combustion chambers. A fundamental property of non-premixed flames is that characteristic lengths are controlled by strain rates. Consequently, the LES mesh resolution in a turbulent flame varies as a function of the local strain rate. A novel approach which aims at controlling the filtered reactive layer size is proposed, irrespective of the local strain rate and mesh size. This approach is developed in the F-TACLES (Filtered tabulated chemistry for LES) framework. To ensure a robust application to diffusion flames, a new gradient-diffusion closure is proposed. A strategy which adapts the local flame filter size is also proposed to control the reactive flame thickness. A posteriori tests are undertaken on 1-D counterflow diffusion flames and the 3-D turbulent coaxial HYLON (Hydrogen Low-NOx) injector. Implementation of the gradient-law closure for the mixture fraction equation proves to be a robust solution in conserving scalar transport of the resolved mixture fraction. The new variable filter size approach outperforms traditional constant filter size cases in predicting the overall flame shape. Since the variable filter uses an optimal filter size, the resolved flame wrinkling is also increased.

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Track04-7 Turbulent combustion (7)

Chair: Fabrizio Bisetti
Friday, May 10; 13:00 - 15:00; Room D

A generic multispecies combustion regime identification for turbulent nonpremixed flame simulations

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Flame stabilization and pollutant emissions are strongly sensitive to the local combustion regime and methods have been discussed in the literature to determine, from numerical simulations, three-dimensional distributions of combustion modes. A complementary approach is proposed to the global regime indexes based on the gradient of reactants, and, to the most advanced indexes requiring the computation of the local chemical explosive modes. This novel method is based on four quantities examining every chemical species present in the simulation in terms of their dynamics versus the spatial distributions of the conserved atomic mass fractions, and their chemical equilibrium conditions accounting for differential diffusion. The atomic-space flame index is grounded on the fact that the atomic concentrations vary much less across premixed and partially premixed flame fronts than across diffusion flame-type reaction zones. The proposed methodology is verified in high-pressure triple-flames propagating around a fuel pocket. The very thin reaction zones under high pressure make the distinction between the combustion modes more challenging. The results confirm the potential of identifying the combustion regimes in the intimacy of complex reaction zones with four parameters related to the conservation of atoms.

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Flame transition in a highly-lifted premixed jet flame in a hot cross flow

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We present a large-scale direct numerical simulation (DNS), with detailed chemistry, of a highly-lifted premixed methane-air jet flame in a hot cross flow, which is relevant to axially staged gas-turbine combustion systems. The simulation features a jet Reynolds number of ~18,000 and a cross flow Reynolds number of ~29,000. The thermo-chemical parameters, except for pressure, closely match those of practical axially staged combustors. In our set-up, a premixed methane-air jet with an equivalence ratio of 0.7 is injected into a vitiated crossflow consisting of combustion products from a methane-air mixture at an equivalence ratio of 0.5, under atmospheric pressure. We analyse this DNS dataset to show flame transition from autoignition to premixed flame propagation, and premixed flame to diffusively supported ignition fronts. While the former phenomenon is due to the interaction between the autoignition kernels and counter-rotating vortex pair, the latter phenomenon is to the accelerated autoignition of the richer mixtures.

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Numerical prediction of blow-out in bluff-body stabilized turbulent flames controlled by thermo-diffusive instabilities

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A Large-Eddy Simulation (LES) study of turbulent flames blow-out taking place in a bluff-body burner is conducted. The present study, utilizing an OpenFOAM-based standard solver for turbulent reactive flows, attempts to predict the blow-out behavior observed in experimental investigations of turbulent premixed CH4-air and NH3/H2/N2-air flames at fuel-lean conditions, and for identical nominal flame properties [1]. In the experiments it was determined that, despite nominally-identical laminar flame characterstics, blow-out occurred at burner velocities differing by an order of magnitude for the different fuels. Localized de-mixing of fuel and oxidiser, hydrogen enrichment of the leading points and subsequent global flame-front acceleration due to thermo-diffusive instabilities cause a significantly-increased resilience to extinction of the NH3/H2/N2-air flames. The physical rate-controlling processes that lead to the observed order-of-magnitude difference in blow-out limits are not conventionally taken into account in turbulent combustion models due to well-known intrinsic limitations. In the present work, utilizing a Partially-Stirred Reactor (PaSR) model jointly with standard LES formulation and unity Le-number molecular transport model, it is shown that the selected model combination is able to accurately capture the blow-out limit for the CH4-air flame but fails to do so for the NH3/H2/N2-air flame. Furthermore, it is also observed that the LES/PaSR predictions of blow-out in the hydrogen-enriched flames can be improved by including a sub-unity Lewis number formulation in the molecular transport model.

[1] S.M. Wiseman, M. Rieth, A. Gruber, J.R. Dawson and J.H. Chen, “A comparison of the blow-out behavior of turbulent premixed ammonia/hydrogen/nitrogen-air and methane–air flames”, Proceedings of the Combustion Institute, vol. 38, pp. 2869–2876 (2021).

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Simulation of attached and lifted swirl-stabilised hydrogen–air flames

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Hydrogen is gaining significant attention, since it is a carbon free fuel. Hydrogen has different characteristics compared to conventional hydrocarbon based fuels, as hydrogen is much lighter and this causes increased hydrogen diffusion compared to thermal diffusion. However, combustion systems have significant challenges with perfectly premixed hydrogen combustion, due to the increased risks of flashback and thermo-acoustic instabilities. Partially premixed combustion is therefore more feasible, but the method of injection of hydrogen needs to be carefully considered to mitigate nitrogen oxide based emissions. A recently developed laboratory scale burner that uses co-axial swirlers ensures quick mixing between hydrogen and air. Altering the mass flow rates at a constant equivalence ratio also leads to different flame archetypes being observed. This work aims to simulate both flame configurations and show comparisons for the flow field and flame shapes with measurements. The interactions between the flow and mixing fields on the flame stabilisation will also be further explored. The flames are simulated using a presumed joint probability density function approach with tabulated chemistry using OpenFOAM.

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Numerical investigation on ignition characteristics of an igniting under-expanded hydrogen jet

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The ignition characteristics of an under-expanded hydrogen jet in a hot ambient atmosphere, corresponding to direct-injection compression-ignition engine conditions, are numerically investigated. Such a hydrogen jet involves significant preferential diffusion, and raises numerical challenges. In the current study, a novel Flamelet Generated Manifold (FGM) method, namely the Projected-FGM, applying an ideal parameterization that spans the local tangential space of the manifold is adopted for combustion modeling and coupled with large-eddy simulation (LES). As a reference, an LES with direct chemistry integration that discards the subgrid turbulence–chemistry interaction is performed. The resulting combustion evolution of the under-expanded hydrogen jet is first compared to available experimental results (Yip et al. International Journal of Hydrogen Energy 45.56 (2020): 32562-32578), and

then analyzed in detail using a variety of approaches. The currently applied Projected-FGM method does not depend on a specifically optimized linear combination of species mass fractions as progress variable, but it solves ordinary transport equations for a few species, which are subsequently projected onto the manifold. It can be applied to any manifold method.

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Track04-8 Turbulent combustion (8)

Chair: Andrew Aspden
Friday, May 10; 15:20 - 17:20; Room D

Large-Eddy Simulations of Fuel Jet Combustion Assisted by the Cylindrical Hot Surface

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This study delves into ignition and flame dynamics with a cylindrically structured hot surface impact incorporated. Previous studies focused on the flat-wall hot surface interacting with fuel spray, but the effects of cylindrical surfaces on fuel-air mixing and ignition have not been fully understood. Using high-fidelity large-eddy simulations (LES), this study reveals physiochemical aspects of reactive mixture elements impinging on an electronically activated glow plug structure. The analysis investigates how the structure enhances fuel-air mixing and affects the low-temperature chemistry of the fuel. To this end, free spray and non-thermal deposit cases are included to inspect the mixing impact. Three different impacting distance are included to differentiate the mixing intensity by altering the impinging spray inertia. Five different electric voltage inputs are also considered to examine the thermally assisted ignition process. Results indicate that the cylindrical structure impedes flow, reducing its inertia and increasing flow residence time. Also, a meaningful Coandă effect is also discovered due to the circular wall structure. Such a mixing enhancement potentially serves as a flame-holding mechanism. In addition, varying the input voltage significantly affects ignition timing. It is an intriguing feature to identify a non-monotonic ignition delay pattern with lower voltages. The detailed analysis discovers the importance of the negative temperature coefficient (NTC) driven low-temperature chemistry (LTC). The further detailed analysis uncovers detailed insights into the physiochemical properties of reactive mixture that contribute to the exothermic ignition pocket formation.

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High-dimensional FGM/ResNet modeling of turbulent spray combustion: Effects of evaporation heat loss and combustion scalar correlation

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In the stratified or partially premixed piloted jet flames, previous experimental and direct numerical simulation (DNS) studies have signified a strong subgrid-scale correlation between mixture fraction and progress variable. In the framework of large-eddy simulation (LES) and flamelet-generated manifolds (FGM) approach, a general joint probability density function (PDF) method is proposed to characterize subgrid correlations. To pave the way for high dimensional tabulation modeling, a deep residual network (ResNet) is trained, dramatically reducing the memory footprint of tabulation. The Message Passing Interface (MPI) shared memory technique is applied to load the 6-dimensional chemical table during parallel computations. Application of LES to a partially pre-vaporized ethanol spray flame demonstrates good agreement with experimental results. Consideration of the subgrid correlation results in a noticeable improvement in temperature prediction. Calculations using ResNet show a notable consistency with those using chemical tables. Visualization of enthalpy highlights the significance of non-adiabatic tabulation in modeling liquid fuel combustion. The impact of the source term due to evaporation in the transport equation of the progress variable is validated. The correlation coefficient significantly influences the chemical reaction rate in the posterior investigation. The subgrid-scale interaction between liquid fuel evaporation and subgrid correlation is elucidated.

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Large-eddy simulation of high-pressure auto-igniting hydrogen injections using tabulated chemistry

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Hydrogen has been labeled for a long time as the fuel of the future due to its carbon-free combustion and the ability to achieve high energy efficiency. The unique

thermo-physical properties of hydrogen can facilitate the design of a highly efficient internal combustion engine (ICE). In particular, direct injection (DI) of hydrogen, aside from enabling high volumetric efficiency, avoids possibly undesired combustion-related phenomena such as engine knock. However, due to its low density, hydrogen requires high injection pressures to fully penetrate in the cylinder.

In this work, we study the combustion process that occurs in high-pressure DI of hydrogen by means of large-eddy simulation with tabulated chemistry, including preferential diffusion. First, the modelling is applied to hydrogen jets in hot air environment for validation against experiments in literature. Then, we investigate different auto-igniting hydrogen jets in a fixed-volume chamber under argon-circulated conditions. In particular, we focus on the effect of ambient temperature and oxygen concentration on ignition delay, heat release rate and flame dynamics.

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Flame structure and stabilisation mechanism of a high-pressure hydrogen micromix combustor

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A high-pressure hydrogen micromix combustor has been investigated using direct numerical simulation with detailed chemistry to examine the flame structure and stabilisation mechanism. The configuration of the combustor was based on a NASA design, using numerical periodicity to mimic a large square array. A precursor simulation of an opposed jet-in-crossflow was first conducted to generate appropriate partially-premixed inflow boundary conditions for the subsequent reacting simulation. The resulting flame can be described as an essentially-lean inhomogeneously-premixed lifted jet flame. Five main zones were identified: a jet mixing region, a core flame, a peripheral flame, a recirculation zone, and combustion products. The core flame, situated over the jet mixing region, was found to burn as a fast thin premixed flame and is responsible for 85% of total fuel consumption, whereas the peripheral flame shrouded the core flame and burned at very lean conditions. It was shown that turbulent flame propagation was an order-of-magnitude too slow to stabilise the flame at these conditions. Stabilisation was identified to be due to ignition events resulting from turbulent mixing of fuel from the jet into mean recirculation of heat. Around the location where ignition was first possible, isolated events were observed, which developed into rapidly burning flame kernels that were blown downstream by the bulk flow. Further downstream, near-simultaneous spatially-distributed ignition events were observed, which appeared more like ignition sheets.

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Soret effect modelling in flamelet-based LES with presumed FDF for lean premixed hydrogen flames

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Soret effect modelling is included for the first time in the framework of turbulent large eddy simulations (LES) with flamelet-based combustion model and presumed filtered density function (FDF) closure for lean premixed hydrogen flames. Preferential diffusion effects are accounted at the thermochemical level with a constant non-unity Lewis number approach, and the diffusive transport of the controlling variables in the LES is corrected accordingly. Within this framework, Soret effect contribution is included on both the diffusive transport of species at the thermochemical level and on the diffusive transport correction of the LES controlling variables. The influence of including or excluding thermal diffusion in the modelling is assessed on a turbulent premixed hydrogen flame in a slotted burner configuration, where favourable conditions for the growth of thermo-diffusive instabilities are established. Results show that, when Soret effect is modelled, the local equivalence ratio redistribution and its coupling with flame front curvature due to preferential diffusion effects are enhanced, and thus a further local increase of reaction rate is observed in correspondence of resolved positively-curved flame fronts. This ultimately affects the macroscopic flame topology, as it triggers an overall increase of turbulent flame speed and thus a decrease of flame jet height.

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Modelling of Spark Ignition Process in High-speed Turbulent Flows using Large Eddy Simulation Based on Strained Flamelet Generated Method

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Due to environmental concerns, lean combustion technology has been widely implemented in spark-ignited in-

ternal combustion engines. In order to enhance the flame propagation under lean conditions, turbulent flows are introduced into cylinders, which leads to unstable ignition processes. This study presents a numerical investigation of spark ignition in lean mixtures under turbulent conditions via Large Eddy Simulation, incorporating a spark discharge model to reproduce the discharge channel behaviors from the calculated electric fields. A strained Flamelet Generated Manifold (FGM) approach was used to reduce the computation cost. Simulations were validated with the results of experiments on a rapid compression machine. Approaches to reduce the computation and interpolation costs in the FGM model were used while considering the accuracy. Results indicated an accurate representation of discharge channel behaviors and motions, including short circuits and restrikes aligning with the experimental data. Flame kernel initiation behaviors, including fragmentation and local quenching effects, were observed and validated with OH* chemiluminescence images from the experiments.

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Track05 Combustion dynamics and instabilities

Track05-1 Combustion dynamics and instabilities (1)

Chair: Abhishek Lakshman Pillai
Wednesday, May 8; 10:40 - 12:40; Room E

Dynamics of hydrodynamically unstable premixed flames in a gravitational field

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Dynamics of hydrodynamically unstable premixed flames with the composite effect of Darrieus-Landau and Rayleigh-Taylor instabilities is investigated. We study the Sivashinsky equation describing time evolution of flame fronts under the small gas expansion assumption and apply the bifurcation theory to extracting a global picture of physically (and nonlinearly) stable flame morphology in various properties of combustible mixture and gravitational environment.

We will see, in the presence of gravitational parameter, (de)stabilization of flame fronts, as well as rich bifurcation structure like hysteresis and splitting/merging behavior of pulsating fronts by means of Hopf bifurcations.

We also investigate the corresponding flame morphology with finite thermal expansion parameter through the hydrodynamic model derived from large activation energy asymptotics, which will provide physically relevant flame morphology observed in the Sivashinsky dynamics.

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Analysis of intrinsic flame instabilities based on entropy generation mechanisms

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Intrinsic flame instabilities, including hydrodynamic and thermodiffusive instabilities, have been analysed based on the statistics of entropy generation mechanisms obtained using Direct Numerical Simulations. The simulations were carried out for two-dimensional laminar premixed planar methane-air flames, with varying amounts of hydrogen addition up to 100% by volume. The mechanisms of entropy generation were analysed based on reversible and irreversible contributions resulting from heat conduction, viscous dissipation, mass diffusion, and chemical reaction. Both qualitative and quantitative methods were used to identify features of the unstable flames. The statistical range of the data dispersion in all entropy generation terms showed periods of growth and reduction, potentially signalling a saturation mechanism. The spatial distribution of all entropy generation terms, except the term due to viscous dissipation, showed the ability to capture the flame front evolution, with some terms indicating the growth and reduction of reactant and product cusps. For the reversible terms, two distinct regions of positive and negative entropy generation rates were observed, while the irreversible terms contributed only positively to the total entropy generation rate. The probability distributions reveal the dominant contribution of the reversible term due to the flux of entropy diffusion to the total entropy generation rate.

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intrinsic instabilities of premixed NH3/H2/air spherical flames under various gravity conditions

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Blending hydrogen into ammonia as a carbon-free fuel has attracted increased attention. However, current understanding of the intrinsic instabilities in premixed NH3/H2/air flames is limited. In the present work, premixed NH3/H2/air spherical flames were performed using direct numerical simulation (DNS). The simulations were conducted under various gravity conditions for the first time to highlight the significant role of Rayleigh-Taylor (RT) instability. A parametric study of spherical flames was performed for different fuel compositions, from pure ammonia to pure hydrogen, equivalence ratios (0.3 to 1.0) and pressures (1 bar to 10 bar). The temporal evolution of spherical flame fronts was investigated in this study, with a particular focus on the flame morphology. The flame displacement speed and its dependence on flame stretch were discussed in detail. The interaction between

Darrieus-Landau (DL) instability, thermal-diffusive (TD) instability and Rayleigh-Taylor (RT) instability was studied to give a comprehensive understanding of the intrinsic instabilities in premixed NH3/H2/air flames.

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A numerical study of premixed laminar ammonia/hydrogen/air flames: an analysis of intrinsic flame instabilities

Ilya Morev, Parsa Tamadonfar, Shervin Karimkashi, Ossi Kaario, Ville Vuorinen
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Blending ammonia with hydrogen may offer a way to control the combustion properties of such fuel mixtures. It is well-known that due to the high diffusivity of hydrogen, hydrogen-containing flames are subject to strong thermo-diffusive instabilities, which results in a significant increase in flame consumption speed. To assess the susceptibility of ammonia/hydrogen/air mixtures to intrinsic flame instabilities, linear dispersion analysis is conducted for a wide range of ammonia/hydrogen blending ratios and equivalence ratios at atmospheric pressure and temperature of 298 K. It is found that mixtures with almost equal molar fractions of ammonia and hydrogen exhibit higher normalized maximum growth rates than pure hydrogen at the same equivalence ratios. Following the linear growth phase, four cases are simulated to reach a fully developed flame front for pure hydrogen and 50:50 ammonia/hydrogen blend and equivalence ratios of 0.5 and 0.7. The resulting increase in the consumption speed compared to the laminar flame speed of the fuel blend with an equivalence ratio of 0.5 is approximately 4, whereas for pure hydrogen, it is around 2.5. This indicates that the overall effect of intrinsic instabilities appears to be larger for this blend, compared to the pure hydrogen case, which also agrees with linear dispersion analysis results.

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Numerical Analysis of Thermodiffusive Instabilities in Fuel-Flexible Methane-Hydrogen Industrial Burner Applications

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The high energy and heat demand of many industrial sectors, e.g., steel production and processing, combined with the need for drastic carbon dioxide emission reductions, requires a transition from fossil fuel industrial burners to novel energy systems in the near future. One widely discussed approach is the utilization of hydrogen. Since hydrogen supply is still limited, industrial burners must be capable of fuel-flexible operation while reducing emissions. However, hydrogen addition to methane strongly influences flame characteristics due to thermodiffusive instabilities.

This study investigates how these instabilities affect the flame in fuel-flexible burners using Large Eddy Simulations (LES). To this end, the model by Regele et al. (Combust. Flame, 160(2):240–250, 2013) is implemented in OpenFOAM. The model is extended for methane-hydrogen combustion to account for instabilities at various operating points including different fractions of hydrogen in the fuel mixture. Subsequently, the model is validated using laminar and turbulent direct numerical simulations (DNS) and experimental data.

Finally, the combustion model is applied to a fuel-flexible industrial burner with complex geometry. Specific features of the burner are the variable hydrogen content in the fuel as well as staging within the mixing unit. The aim is to understand the effect of thermodiffusive instabilities in a realistic application at different operating conditions. For this, temperature distributions, NOX emissions, and flame stability limits are analyzed.

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Track05-2 Combustion dynamics and instabilities (2)

Chair: Hong Im
Wednesday, May 8; 13:30 - 15:10; Room E

Numerical investigation in canonical flat V-shape propagative reactive fronts

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To prevent accidents related to hydrogen utilization, it is crucial to enhance our understanding of the early stage of reactive front accelerations. In this context, we propose a canonical numerical setup to investigate the mechanisms involved in the interaction of two reactive fronts, which may result in sudden accelerations of flames or auto-ignition fronts.

The proposed configuration, designed to facilitate physical analysis, requires meticulously controlled initial conditions - a challenge often difficult to overcome in practical experiments.

The investigation focuses on low Mach interactions and is conducted using the DNS solver – PeleLMeX-,

which integrates Adaptive Mesh Refinement (AMR). The initial condition is crafted using a reduced chemical mechanism and the CANTERA library through laminar flame simulations or a series of homogeneous reactor computations. These preliminary calculations provide the initial temperature fields yielding a constant propagation speed of reactive fronts.

The studied configuration is 2D, and the two impacting reactive fronts are flat, resulting in a V-shaped front where the collision angle serves as a crucial parameter in the analysis. As anticipated, the initially flat V-shape of the fronts evolves over time due molecular diffusion interactions. The curvature of the front formed at the point of impact gradually adjusts, in some cases leading to local accelerations.

This study aims to provide new insights into the effects of reactive front properties (such as initial propagation speed, collision angle, etc.) on the propagation dynamics and accelerations.

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Characteristics of transverse flame describing functions of slot and Bunsen flames at large amplitudes

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In this study, G-equation simulations were conducted to characterize the transverse flame describing functions (FDFs) of slot and Bunsen flames under imposed transverse velocity fluctuations across various frequencies. The simulations were validated by analytical models at low amplitude conditions: longitudinal acoustic forcing of Bunsen flames and transverse acoustic forcing in slot flames. Simulations are conducted with a mean transverse velocity as the transverse FDFs are zero without the mean transverse velocity due to flame symmetry. For slot flames, the FDF gains asymptotes to zero at low frequencies and increase right after. Still, the overall envelop of the gains decreases with frequency, illustrating a typical low-pass filter behavior. At large amplitudes, the FDF gains increase with larger than the low amplitude conditions. Bunsen flames displayed a similar trend but with notably lesser gain magnitudes. The small gain is attributed to the different mean flame shapes, which are linked to heat release fluctuations. Understanding the difference in gain of FDFs is crucial for comprehending flame dynamics related to transverse acoustic effects. A comprehensive FDF modeling including both longitudinal and transverse forcing are necessary to predict combustion instability.

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Effect of central recirculation zone on the instability growth in a V-shaped swirling flame

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This paper presents a numerical and theoretical study on the instability growth in a V-shaped swirling flame, with an emphasis on the effect of varying central recirculation zone (CRZ). First, the basic unsteady flame and flow characteristics are studied using large eddy simulation (LES) with the flamelet generated manifold (FGM) model. The resultant velocity profiles, flame structures, and vorticity distributions show good agreement with the corresponding experimental data, confirming the validity of the numerical approach. Then, a linear spatial stability analysis is performed based on the simulated mean flow to study the growth of small disturbances. With the CRZ size varied through tuning the equivalence ratio (φ), the growth rate of axisymmetric disturbance shows a decreasing trend with increasing CRZ size, whereas the growth rate of asymmetric disturbance increases with the CRZ size. By further analyzing the source terms in the Reynold-Orr equation, we find that the growth of axisymmetric disturbance is dominated by the axial velocity shear, whereas the growth of asymmetric disturbance is governed by the combined effects of axial and azimuthal velocity shears.

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Vorticity transport of the precessing vortex core in a premixed swirling flame

Qiuxiao Wang, **Xi Xia**, Fei Qi
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This work numerically explores the mechanism governing the intensity of the precessing vortex core (PVC) in a premixed swirling flame of the helical mode. Large eddy simulation (LES) together with the flamelet generated manifold (FGM) model is employed to understand the dynamical interaction between the spiral flame surface and flow field. The validation of the numerical approach is performed based on comparisons of the simulated velocity field and flame structures with the experimental results. To quantify the local intensity of the PVC, the circulation, Γ, is computed in the plane perpendicular to the PVC tube axis. We find that $|\Gamma|$ first increases along the PVC winding direction and then decreases upon reaching a peak value. To explain the variation trend of $|\Gamma|$, vorticity transport analysis is performed within a local control volume enclosing the PVC element. The results reveal that both vortex stretching/tilting and baroclinic torque contribute to vorticity growth in the PVC, whereas thermal dilation

and vorticity diffusion cause the PVC intensity to decay. This understanding supplements the existing knowledge regarding the formation and spatial development of PVC in swirl combustion.

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Track05-3 Combustion dynamics and instabilities (3)

Chair: James Dawson
Wednesday, May 8; 15:30 - 17:10; Room E

The dynamics of a cellular flame deformation from the head on interaction with an expansion wave

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We address the problem of cellular flame deformation after a head-on interaction with an expansion wave. Our focus is on studying the wrinkling behavior of hydrogen-air flames and examining the influence of the Lewis number on the dramatic flame deformation resulting from the interaction. This problem is addressed numerically by direct numerical simulations of the reactive Navier-Stokes equations in 2D, using a single-step Arrhenius law. The physical mechanism of deformation is established to be through the baroclinic vorticity production mechanism, augmented by the gas expansion during deformation. It is found to be similar to but more efficient than the flame deformation by the passage of a shock with the same overpressure (Yang and Radulescu, JFM 2022), due to the longer residence of the flame in the region of vorticity deposition. The effect of the lower Lewis number for lean flames was found to provide an increase in flame deformation and burning rate enhancement as compared to stoichiometric unity Lewis number flames. This is due to the higher propensity of curved flames to further deform through the thermal-diffusion instability mechanism. The flame deformation dynamics were monitored for different expansion strengths and distances from the flame, originating from either the burned or unburned side. Nonlinearity, and the competition between pressure gradient magnitude and residence time were found to play subtle roles in the deformation dynamics. A model was proposed to predict the evolution of the flame burning rate for arbitrary expansion wave and flame properties.

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Influence of numerical damping on the prediction of high-frequency thermoacoustics and mitigation strategies for LES

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Thermoacoustic instabilities limit the operating range of gas turbine combustors, impeding further efficiency gains and emission reductions. The prediction of instabilities can be achieved with compressible large-eddy simulations (LES), which considers all physical mechanisms of thermoacoustic processes. Notably, the numerical methods employed in LES damp the propagation of pressure waves, leading to a non-physical loss in amplitude over time and space. The numerical damping depends on the spatial and temporal resolution of the waves, leading to higher damping for higher frequencies. In this work, the impact of numerical damping on the prediction of high-frequency thermoacoustics is studied. Highly-resolved compressible, reactive LES of a self-excited high-frequency atmospheric model combustor are carried out. The results show that higher numerical damping reduces the limit-cycle amplitudes significantly, and can even stabilize the case, resulting in no HFI prediction. The influence on mode shape and frequency of the unstable acoustic mode is small for the considered cases, if HFI occurs. The results indicate that the numerical damping acts as a suppression of HFI. Possible mitigation strategies to recover the prediction of HFI on meshes with higher damping are discussed and a method based on the amplification of thermoacoustic flame response is presented.

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Combustion Characteristic Analysis of the Dual Combustion Ramjet Engine

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The investigation of combustion characteristics in the Dual Combustion Ramjet (DCR) engine is undertaken through a numerical study employing a Large-Eddy Simulation (LES) approach, with detailed chemistry and species conservation equations. Two distinctive combustion modes are discerned under the same inflow condition but with varying initial conditions. In supersonic shear layer combustion, the initial condition is given 1,200K air. The thermally choked mode is observed in 3,200 K air, which is artificially assumed to have increased the initial temperature due to certain non-ordinary events. These modes

emerge due to compressibility effects, turbulent motion, pressure waves, and heat addition. The findings imply that mode control in the DCR is attainable through the strategic introduction of critical heat addition or ignition sources.

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Flamelet modeling of curvature effects on NOx formation in thermodiffusively unstable premixed hydrogen flames at elevated-pressure conditions

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Fuel-lean premixed hydrogen flames are thermodiffusively unstable and burn in cellular structures due to strong differential diffusion of hydrogen. Pressure promotes the thermodiffusive instabilities due to the increase in Zeldovich number and the relevant reaction pathways. As the local stochiometry and temperature correlate with the thermodiffusive instabilities, the NOx formation mechanism is expected to be complicated in fuel-lean hydrogen flames at elevated-pressure conditions. Furthermore, the thermodiffusive instabilities correlate with the curvature of the flame front, the NOx formation are expected to be affected by the curvature. To consider the effects of curvature, an extended flamelet tabulation method based on the composition space model (Scholtissek et al., CNF, 2019) is proposed. The performance of the composition space model in predicting the NOx species is evaluated using a posteriori} simulations. The simulation results obtained with the composition space model will be compared with the reference DNS data and the flamelet model proposed by Regle et al.~(CNF, 160 (2013) 240-250), in which the curvature is considered by varying the equivalence ratios. We will focus on thermodiffusively unstable premixed hydrogen flames at elevated-pressure condition (8\,atm) for different equivalence ratios.

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Track05-4 Combustion dynamics and instabilities (4)

Chair: Michael Gauding
Thursday, May 9; 09:50 - 12:30; Room D

Bifurcation dynamics of lean hydrogen flames in narrow channels

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Very lean hydrogen-air mixtures confined in slender channels have been recently found to produce bistable fronts, either circular or double-cell flames. In particular, these two stable configurations arise for the same combination of controlling parameters (equivalence ratio, channel size and thermal conductivity) in the limit of fuel-lean mixtures and non-negligible conductive heat losses. In this study, numerical experiments are performed to detail the unsteady evolution that forms either one structure or the other during a particular ignition transient and provide a satisfactory explanation of their symmetry-breaking dynamics.

We offer causality analyses based on the initial temperature profiles (hot-region distribution and peak value) and subsequent expansion of the flow field, which prescribe the early growth of the flame front leading to different curvatures and sizes of the kernel. These processes control the evolution into each of the canonical structures owing to the underlying physics. Specifically, differences in the local convective effects and interactions between fronts have been identified as the key causes to produce each of the final-stage bistable fronts.

In fact, frequently found fragmentation of flames cannot ensure the formation of double cells, which require additional reorientation dynamics of the subdivided parts to achieve their coupling. The reorientation process is produced through asymmetric seeding of flame fragments or to the interaction with neighboring structures, which are particular events very dependent on the ignition configuration.

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LES of wet hydrogen combustion in a counter-current nozzle configuration

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Employing Large Eddy Simulations (LES), we investigate nitrogen-diluted hydrogen flames in a counter-current configuration in which a fuel nozzle is embedded in a larger annular nozzle sucking the fluid from the surrounding of the fuel jet. Such an injection system produces a counterflow in the vicinity of the nozzle, which is beneficial for triggering global instability. The research explores the interactions between global instability phenomenon, fuel-oxidizer mixing, and flame-stabilization mechanism, crucial for enhancing technical efficiency and environmental sustainability. The flames are ignited through the energy deposition model. The primary focus is on the impact of spark position, suction strength, and water-vapor dilution on the flame stabilization mechanism. During the transition to global instability, toroidal structures and side-jets emerge, enhancing fuel-oxidizer mixing and simultaneously preventing the flame attachment to the nozzle. The study also highlights the impact of water-vapor dilution on ignition and flame stabilization following the current trend of wet combustion technique. The water-vapor presence hinders ignition and contributes to lifted flame stabilization. The coexistence of global instability and water-vapor dilution offers novel insights into flame stabilization mechanisms, presenting opportunities for optimizing combustion systems and advancing safety and efficiency.

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LES of an excited hydrogen flame stabilised by cylindrical and star-shaped bluff bodies

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This research focuses on the dynamics and stability of a nitrogen-diluted hydrogen flame formed downstream a bluff body with a cylindrical and star-shaped wall positioned in an oxidiser duct. To intensify the mixing process an excitation is imposed on an oxidiser mass flow stream. The study employs the Large Eddy Simulation (LES) method, providing detailed insights into the intricate physics of unsteady flow. The main goal of the research is to assess the impact of bluff-body shape and excitation parameters (frequency, amplitude) on the formation of large and small-scale vortical structures and to analyse how their alteration influences flame parameters (flame shape, fuel consumption, temperature and species distribution). We found that in the case of the cylindrical bluff body, the mixing process is driven by periodically generated large toroidal vortices resulting from Kelvin-Helmholtz instability. Applying the excitation enhances the formation of these vortices and leads to an intense transport of oxidiser into the recirculation zone. On the contrary, the star-shaped bluff body induces azimuthal disturbances that prevent the formation of toroidal vortices. Instead, small high-frequency vortices are generated. They foster intense small-scale mixing leading to a flame elongation and a more uniform temperature distribution. Its maximum level is decreased by approximately 200 K, which may have a significant impact on the thermal reduction of NOx.

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Large-eddy Simulation of flashback of lean-premixed low-swirl hydrogen jet flame

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Lean-premixed hydrogen combustion is currently attracting attention as an eco-friendly strategy for use in aircraft gas turbine engines. This method has the advantage of emitting no CO_2 and significantly reducing NOx emissions by lowering the flame temperature. Despite this advantage, flame flashback into the injector is one of the underlying problems of premixed hydrogen combustion. As flashback damages the combustor system and harms the safe operation of the gas turbine engine, investigation of the flashback mechanism is crucial. This study analyzes the flashback of a lean-premixed swirling hydrogen flame in a low-swirl combustor (LSC) using Large-eddy Simulation employing the dynamic Smagorinsky Model as a subgrid turbulence model. The dynamically thickened flame model is also applied as a turbulent combustion model to resolve the flame thickness on the LES computational grid. The presented results show that flashback is initiated from the center of the injector after the lifted flame attaches itself to the periphery of the injector exit. This type of flashback is specific to the flow field in LSC, where the mean velocity away from the LSC axis is larger than that at the LSC axis. Flame dynamics and flame propagation characteristics during flashback are also investigated.

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A study of dynamic thickened flame modeling effects on intrinsic instabilities of premixed hydrogen flames in comparison with direct numerical simulations

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Laminar premixed lean hydrogen flames are thermo-diffusively unstable, which leads to significant flame front wrinkling and faster flame propagation compared to that of the laminar unstrecthed burning velocity. On the other hand, hydrogen flames have very thin interfaces, making their modeling challenging. The thickened flame model targets at manipulation of the governing equations so that the flame front is artificially thickened without affecting other characteristics of the flame. This study explores the effects of artificial flame thickening on intrinsic flame instabilities numerically. The open-source CFD toolbox OpenFOAM is used together with a dynamic load-balancing library (DLBFoam), where the dynamic variant of the thickened flame model is implemented. The results show that similar intrinsic instabilities, observed using direct numerical simulations (DNS), are obtained when the thickened flame model is used. However, the length and time scales of these instabilities are stretched by the thickening factor. This leads to slower developments of the flame fingers and thus, slower consumption speeds during the flame front development, compared to the DNS results, while the final consumption speeds remain approximately the same.

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High-fidelity Large-Eddy Simulations of ignition of lean H2/air flames: Unveiling the role of hydrogen diffusivity and extinction strain rate on the flame dynamics

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High-Fidelity LES are used to unveil the influence of hydrogen diffusivity on the flame dynamics during ignition of lean H2/Air flame. The simulations cover a CH4/air mixture with a unity Lewis number and a lean H2/air mixture with a sub-unity Lewis number. Both mixtures are injected at a fixed bulk flow velocity of Ub = 5 m/s, with the equivalence ratio adjusted to match the laminar unstretched flame speed of S_l= 0.25 m/s. The numerical setup is first validated against isothermal and reactive PIV measurements, as well as OH-PLIF images, showing a very good agreement. Analysis of the absolute flame speed S_a revealed that despite its lower thermal expansion ratio (ρ_u/ρ_b), the H2/air flame a higher absolute flame compared to the CH4/air mixture. It was further demonstrated this dynamic is promoted by the interplay between thermal expansion and stretch effects evaluated via the stretch factor I_0. While CH4/air flame has a higher thermal expansion ratio, the H2/air flame displayed higher I_0 values due to the effects of preferential diffusion. Expanding the examination into a local analysis of the flame front dynamics during flame expansions that the extent of flame propagation into the high shear flow regions is governed by the local flame stretch. Excessive stretch values often result in flame quenching, particularly evident in CH4/air flames where the critical threshold value is notably lower. In contrast the high resistance to stretch of H2/air flames allows the combustion reaction to persist in those region, facilitating widespread flame expansion throughout the entire domain.

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Numerical Study on Controlling Factors Affecting Flow Dynamics of Combustion Gases in Municipal Solid Waste Incinerators

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At several municipal solid waste incineration facilities in Fukushima Prefecture, the incinerators are operated manually, so waste combustion can be affected by differences in operating techniques among the incinerator operators. In particular, the plastic waste, which has been increasing in recent years, burns with a high calorific value, and there is concern that a sudden increase in combustion gas temperature may damage the inner walls of the incinerator. Therefore, as part of a study to minimize the influence of operating techniques on the incinerator operation and to enable stable operation under transient combustion conditions, evaluation of combustion behavior in the incinerator through a numerical simulation was considered. In this study, sensitivity analyses were conducted under conditions that simplified the specifications of the municipal solid waste incinerator in operation in Fukushima Prefecture, using as parameters the controlling factors that affect the combustion gas flow dynamics in the incinerator. The controlling factors were the amount of fuel

waste supplied to the incinerator and the air flow rate injected into the incinerator to promote combustion. As a result, the combustion gas flow distribution and combustion gas temperature distribution in the incinerator were qualitatively predicted. The results of the present study quantitatively clarified operating conditions that can maintain the combustion gas temperature in the municipal solid incinerator below the upper limit (900-950°C) even for transient combustion conditions.

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Track06 Emissions and pollution

Track06-1 Emissions and pollution (1)

Chair: Stelios Rigopoulos
Wednesday, May 8; 15:30 - 17:10; Room L

Manifold modeling for reactive nitrogen emissions in ammonia-hydrogen-nitrogen turbulent nonpremixed flames

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The use of ammonia as an alternative fuel is challenging due to the need to minimize reactive nitrogen (nitrogen oxides and nitrous oxide) emissions. In gas turbine-like configurations, recirculating flows increase residence times allowing for the reduction in unrelaxed emissions, which have been recently pointed out as the major contributor of reactive nitrogen emissions. To gain further insight on the impact of residence time on reactive nitrogen emissions, a laboratory-scale ammonia-hydrogen-nitrogen turbulent nonpremixed bluff body flame is investigated using Large Eddy Simulation (LES) employing a manifold model for nonpremixed combustion. Results are validated against experimental measurements. Extensive analysis is carried out to understand the influence of the manifold model assumptions in predicting reactive nitrogen results. Unlike in hydrocarbon combustion where the formation of reactive nitrogen emissions is almost always slow and in small concentrations, reactive nitrogen emissions in ammonia combustion form and relax over a range of chemical time scales and can be present in large concentrations. Therefore, a new manifold model formulation is proposed, termed a partially non-equilibrium manifold formulation, in which chemical species governed by slow chemical time scales are solved using a non-equilibrium manifold formulation, which, to ensure mass consistency, constrain the chemical species governed by fast time scales and an equilibrium manifold formulation.

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Numerical investigation and modeling of NOx emissions during ignition and combustion of pulverized biomass fuels

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In order to develop reduced-order models for the correct prediction of NOx emissions in pulverized biomass flames, NOx formation pathways in biomass combustion in air and oxy-atmospheres are investigated by direct numerical simulations. Solid biomass fuels contain fuel-bound nitrogen, which contributes to NOx formation and complicates the NOx prediction. The NOx formation pathways and modeling of NOx emissions in biomass combustion are not fully understood, necessitating further investigation through detailed kinetic models. Therefore, reactive biomass simulations in a hot co-flow configuration in laminar conditions considering the detailed NOx surrogates are performed. To this end, the detailed CRECK-S kinetic scheme for the solid-phase and a newly developed detailed gas-phase kinetic model, including the NOx formation pathways for biomass combustion, are employed. NOx formation is very sensitive to several parameters in solid pulverized fuel flames, such as solid fuel type and composition, particle size, particle injection rate, and ambient conditions. The current study assesses the effects of these different parameters on the formation of NOx pollutants. In particular, a detailed pathway analysis is performed to identify the contributions of fuel-related NOx and thermal NOx emissions. Finally, based on the analysis of the NOx formation pathways and the identification of the dominant pathways at different conditions, guidelines for reduced-order modeling approaches for the correct prediction of NOx pollutants are discussed. To this end, detailed simulation results are utilized to identify the suitable parameters to describe the particle-chemistry-pollutant interactions in the context of tabulated Flamelet models through an optimal estimator analysis.

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Numerical simulation of hydrogen-air-steam flames with NOx production

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The use of hydrogen (H2) as an alternative fuel to hydrocarbons constitutes a major challenge to reach carbon neutrality. However, operating an engine with hydrogen is a difficult task since hydrogen, a molecule with a low molecular weight, is highly flammable in the air with a fast chemical kinetic and high combustion temperature. This leads to scientific and technological issues such as pre-ignition and engine knocking, flashback, flame stabilization, transition to detonation as well as polluting emission of nitrogen oxides (NOx). To overcome the difficulties associated with H2/air combustion, steam dilution combustion appears as a promising approach to decrease the flame speed, the adiabatic flame temperature, and the NOx emission. Understanding and predicting hydrogen-air-steam flame structures are therefore major issues in the context of high-fidelity simulation which are presently studied through jet flame configurations to highlight the importance of detailed chemical schemes, preferential diffusion, exhaust gas recirculation, and flame wrinkling in NOx production. The role of species NNH has been scrutinized since it is a pivotal species for NO creation.

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A direct numerical simulation study of wet combustion effects on NOx/N2O formation pathways in laminar and turbulent premixed ammonia/hydrogen/air flames

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While ammonia/hydrogen combustion offers a great potential to facilitate a smooth transition to clean combustion, NOx/N2O mitigation in such flames is of great importance. In this work, direct numerical simulations of planar premixed ammonia/hydrogen/air flames are conducted under laminar and turbulent conditions in OpenFOAM using detailed chemistry. First, under laminar conditions, a study utilizing parametric sweeps of the equivalence ratio (φ), steam-to-air ratio (Ω), and ammonia/hydrogen blending-ratio (α) pinpoints conditions associated with reduced NOx/N2O emissions while ensuring that flame properties remain pertinent to those observed in hydrocarbon flames. Second, effects of isotropic homogeneous turbulence in the thin reaction zones regime for three cases are studied and NO formation pathways are thoroughly investigated. Under both laminar and turbulent conditions, wet combustion (Ω~0.3-0.5) leads to NO emissions drop by a factor of 2-3 compared to the dry cases at similar (φ, α). The main reason for NO mitigation by adding steam is found to be (i) lower combustion temperature, and (ii) switches in the NO formation pathways, mainly attributing to the reduced contribution of HNO pathway in producing NO and the amplified share of N2 and N2O pathways in consuming NO. Moreover, the role of individual reactions in pathways switches is analyzed.

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Development and performance analysis of a novel, energy-efficient PNG porous burner for cooking applications

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Cooking requires a substantial amount of energy. In growing countries like India, the primary energy source for cooking applications is liquid petroleum gas (LPG). There are notable challenges associated with LPG, including the risk of leakage, which can lead to major accidents due to its highly flammable nature, and the need for cylinder refilling when it is drained. In the current investigation, piped natural gas (PNG) is considered a promising alternative with continuous fuel supply for cooking applications. It is recognized as a cleaner-burning fuel that produces lesser greenhouse gas emissions (CO2, NOx) and particulate matter (soot) during combustion, contributing to a lower environmental impact. Based on the literature, in the present study, the porous domain is considered for flame stabilization under fuel lean operating conditions and to facilitate internal heat recirculation, thereby preventing local quenching. The numerical study is conducted to analyze the performance and emission characteristics of a novel energy-efficient porous burner (NPB) operated on PNG (95% CH4 and 5% C2H6) for different thermal inputs (1-3 KW) using the reduced USC Mech_50 species chemical kinetic mechanism and compared with the conventional LPG burner (CB). The developed novel burner demonstrated stable combustion inside the porous domain over entire operating conditions. In comparison to a CB, a notable increase in thermal efficiency, reaching up to 3%, along with significant reductions in CO, CxHy, and NOx emissions of an NPB is observed.

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Track06-2 Emissions and pollution (2)

Chair: Nozomu Hashimoto
Friday, May 10; 15:20 - 17:40; Room G

Effect of oxygenates on soot formation during the combustion of fuel-rich CH4 mixtures

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Polygeneration in internal combustion engines enables a variable generation of mechanical power and valuable chemicals based on reactions under fuel-rich conditions depending on the fuel/air equivalence ratio phi= and the reaction conditions. This may help to mitigate one of the main challenges of future energy systems – accommodating fluctuations in energy supply and demand. Investments in devices for grid stabilization could be more economical if they have a second use. For conversion of ultra-rich fuel/air mixtures into potentially useful chemicals in a polygeneration context, oxygenated compounds are of interest to increase fuel conversion while suppressing soot formation. Thus, the influence of various oxygenates (diethyl ether (DEE), methanol, or dimethoxymethane (DMM)) on soot formation was addressed by studying the oxidation (phi=5 of gas mixtures using CH4 as base fuel and additives (10 mol% relative to the base fuel) in a shock tube at 1480–1900 K at around 5 bar. Laser extinction at 633 nm was used to measure soot optical densities and absorption spectroscopy with mid-IR quantum cascade lasers yielded temperature and CO concentration as a function of reaction time. Experimental data is compared to simulations.

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Effects of Hydrogen and Ammonia Substitution on Soot Formation in Turbulent Ethylene/Nitrogen Jet Flames

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This study investigates the effects of hydrogen and ammonia addition on soot formation in turbulent non-premixed ethylene/nitrogen jet flames. Large Eddy Simulations with the Flamelet/Progress Variable (FPV) model, considering comprehensive soot-turbulence-chemistry, are conducted. A detailed chemical mechanism including heavy PAH like coronene is used to explore the influence of varying hydrogen and ammonia concentrations on PAHs. The effects of hydrogen or ammonia doping on temperature, different species (such as HCN and benzyl radical), and their impact on soot formation source terms, including nucleation, surface growth, condensation, and oxidation are explored, revealing the complex interactions that ultimately influence soot formation. It is found that consistent with the experimental results, introducing hydrogen increases soot volume fraction, whereas ammonia doping has the opposite effect. Notably, ammonia addition significantly suppresses the formation of heavy Polycyclic Aromatic Hydrocarbons (PAHs). The addition of ammonia substantially impacts the surface growth process, impeding the further growth of soot particles.

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Modal analysis of flow dynamics and soot evolution in an aero-engine model

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Soot formation and evolution are very sensitive to flow dynamics encountered, especially in confined turbulent swirling flows where strong shear layers and recirculation regions will introduce fast time-scale and slow time-scale complex coherent patterns. These patterns are frequently essential to unlock our understanding of soot evolution and to control soot formation and emission. To this end, large-eddy simulations (LES) of an aero-engine model combustor with and without dilution jets are conducted with state-of-the-art soot models. Then, modal analysis of flow and soot dynamics in the combustor is performed using the spectral proper orthogonal decomposition (SPOD) method with transient LES data. The frequency bands of both high-frequency dynamics (HFD, 234.375-468.75 Hz) and low-frequency dynamics (LFD, 0-156.25 Hz) are identified. It is found that compared to LFD, the HFD has a major impact on velocity and PAH, while LFD plays a critical role in soot evolution. This is because the impact of HFD exhibits an energy transfer process, i.e. velocity HFD affects PAH, and then PAH would transfer modal energy to soot. However, the evolution of velocity, PAH, and soot are found to be closely coupled with each other within the LFD frequency band. Furthermore, it is found that for soot and PAH, the impact of dilution jets on HFD modes is minor and on LFD modes is significant, while the opposite impact is observed on velocity modes.

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Numerical Computation of Sooting Flames with a New Soot Fusing Model

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The prediction of sooting flames is a formidable challenge due to the need to account for several complex kinetic processes and their interaction with fluid dynamics. In this work, we focus on the fusing of soot aggregates, for which a new model is presented and investigated via the numerical simulation of a series of laminar co-flow diffusion (Santoro) flames. To predict the morphology of aggregates, a coupled two-population balance model that solves for the distributions of aggregates and primary particles is employed and integrated within a computational fluid dynamics (CFD) code. This allows for the inclusion of a finite-rate timescale for fusing, a process that increases the primary particle size. A new model for the fusing timescale, derived from carbon black reactor data, is presented and employed in the context of the two-population balance approach. Simulation results are compared against experimental measurements for three Santoro flames, namely a non-smoking, an incipient smoking and a smoking flame, as well as against simulations employing fusing timescales obtained from expressions based on silica and titania models. It is found that the fusing rate has significant influence when predicting the quantity of soot escaping the flame as smoke.

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An LES-PDF-DPBE method for the flow dynamics and soot formationin in an aero-engine model combustor: an insight into the soot micromixing requency

Anxiong Liu, Kun Luo

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This work presents the LES-transport pdf-discretised PBE approach to model fluid dynamics and the evolution of soot particles in a pressurised swirling-flow aero-engine combustor. This approach considers the interaction between turbulent reacting flow and soot particles. A reduced chemical kinetics mechanism including a series of PAHs species linked to soot formation is generated employing the DRGEP approach, and is tested on a perfectly stirred reactor under varying equivalent ratio conditions. The soot kinetics model includes the PAH-based nucleation and surface condensation, the HACA surface growth and oxidation mechanism, and the size-dependent aggregation. The soot morphology considers geometrical properties for both spherical primary particles and fractal aggregates. The simulation results show generally good agreement with experimental measurements in terms of swirling vortex, flame shape, temperature, OH species, and soot volume fraction. By increasing the equivalence ratio at the primary injector, the influence of the low frequency dynamics on soot formation is decreased.

A single micromixing frequency is usually taken for both particulate soot and gaseous species, which is not physically correct due to the much smaller molecular diffusion of soot than gaseous molecules. To investigate the effect of the soot micromixing, a quantitative analysis is conducted by reducing the micromixing frequency factor from 1.0 to 0.1. The maximum soot volume fraction is observed to increase a bit. However, compared with the soot modelling using different soot kinetics and numerical methods (like other LES and RANS simulation references), the difference of the soot predictions by varying the soot micromxing frequency is negligible.

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NUMERICAL INVESTIGATION ON THE FUEL FLEXIBILITY OF A TYPICAL AERO-ENGINE SWIRL-STABILIZED FLAME

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In science and industry, swirling flows are found in a wide range of applications. In combustion, it is commonly used to stabilize a flame. It maintains its ignition by recirculating the burnt gases with the incoming fresh air and fuel. Depending on the swirl intensity, residence times may vary in the hot areas and thus, it tends to limit NOX formation. In the context of reducing emissions of aviation gas turbine engines, various sustainable aviation fuels are being developed with the aim of keeping the existing infrastructure unchanged. Thus, considering the variety of fuel alternatives for aeroengines being increased, there exists a clear demand for characterization of the fuel behavior and flame interactions with the highly turbulent flows found inside such combustion chambers.

The Triple Annular Research Swirler (TARS) burner, that mimics aeroengines combustors, has been previously employed for experimentally studying non-reactive and reactive flows dynamics in open and confined combustion chamber conditions. Here, combustion Large Eddy Simulations are used to investigate the combustion dynamics of kerosene-based liquid jet fuels such as Jet A but also test fuels such as C1 and C5. The simulation results

are analyzed in comparison with the experimental data acquired during the measurement campaigns, which includes OH* chemiluminescence, OH* planar laser induced fluorescence (PLIF) and particle image velocimetry (PIV).

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Novel multiscale modeling methodology for chemical kinetic modeling of fuel oxidation using atomistic calculations: Application towards hydrogen combustion

Bhuvan Raj Maddipati, Aditya Konduri, Phani Sudheer Motamarri
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Chemical kinetic (CK) models are indispensable for high-fidelity continuum-scale combustion simulations, providing detailed insights into flow-chemistry interactions. Contemporary approaches to CK modeling combine experimental data with theoretical calculations, such as transition theory, to construct a reaction mechanism that is further validated based on experimentally obtained flame speeds and ignition delay times. Despite extensive experimental validation, these highly parameterized CK models are only valid for a specific range of temperatures and pressures and eventually fail at extreme conditions (e.g., thermodynamic non-equilibrium). In contrast, reactive molecular dynamics (RMD) offers a promising solution that can incorporate the intricacies of extreme conditions and provide a necessary CK model. By facilitating ReaxFF-based molecular dynamics, RMD offers a distinctive advantage, enabling the direct exploration of pathways, identification of intermediates, and calculation of reaction rates, surmounting the limitations associated with conventional techniques. Recent studies have explored CK modeling using the canonical ensemble, which, however, falls short in providing sufficient information and computationally expensive. In this study, the reaction mechanism and rate constants of the hydrogen-oxygen system are computed using microcanonical ensembled RMD trajectories. Arrhenius parameters are fitted for each elementary reaction by computing the kinetic rates at various temperatures, and a comprehensive CK model is developed for hydrogen oxidation. The accuracy of the MD-derived parameterization is assessed by examining the flame speed in one-dimensional premixed continuum-scale simulations and comparing the results to standard values. A consistent agreement in flame speed is observed across various equivalence ratios, underscoring the robustness of the information derived from RMD simulations.

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Track07 Droplets and sprays

Track07-1 Droplets and sprays (1)

Chair: T.-W. Lee
Wednesday, May 8; 10:40 - 12:20; Room C

Numerical study on preferential evaporation characteristics of ATJ-SPK/ Jet A spray flames in laminar counter-flow

Yanqi Zhang, Zhenhua An, Jiangkuan Xing, Ryoichi Kurose
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Abstract: Sustainable aviation fuels (SAFs) play an important role in the goal of achieving carbon neutrality in the aviation industry by 2050. Currently, SAFs are allowed to be used by blending with conventional aviation fuels up to certain percentages. Understanding the spray flames of the fuel blends is crucial for their clean and efficient utilization in aircraft engines. In this study, direct numerical simulations of laminar counter-flow spray flames are performed. The fuel is the 50%-50% blend of ATJ-SPK and Jet A. The Hychem mechanism is used to account for the gas phase combustion. The preferential evaporation behavior is investigated under three droplet sizes (20, 40, and 70μm) and three strain rates (50, 100, and 200 1/s). The numerical results indicate that the droplet size and strain rate determine the droplet penetration into flame fronts, which ultimately influences the intensity of the preferential evaporation. Overall, at high Stokes numbers. strong effects of preferential evaporation can be observed in reaction zones, which can influence the local fuel composition and the subsequent combustion behavior of spray flames.

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Artificial Neural Network Aided Vapor-Liquid Equilibrium Model for Multi-Component High-Pressure Transcritical Flows with Phase Change

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To enhance efficiency in modern combustors, elevating system operating pressure is common, often leading to supercritical and transcritical fluid regimes. The first principled Vapor-Liquid Equilibrium (VLE) model for transcritical thermodynamic modeling is computationally intensive and has encounters robustness challenges. This study introduces a novel Artificial Neural Network (ANN)-aided VLE model for fully compressible CFD solvers. The ANN, trained in Python with TensorFlow and optimized for inference using ONNX Run-time, can integrate seamlessly with any C++-based compressible CFD solver. This plug-and-play model enables simulations of transcritical processes in high-pressure liquid-fueled propulsion systems using only open-source packages, eliminating the need for proprietary VLE model development. The model's performance is evaluated in shock-droplet interaction and temporal mixing layer simulations, surpassing performances of direct evaluation and the in-situ adaptive tabulation (ISAT) method. Notably, it demonstrates implicit load balancing and robust strong parallel scalability. The plug-and-play methodology is versatile, as demonstrated by coupling it with an open-source real-fluid CFD solver to study high-pressure droplet evaporation at liquid-fueled detonation conditions. This approach addresses computational challenges in transcritical thermodynamics while offering a flexible solution applicable to various compressible and conservative CFD solvers.

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Multi-component evaporation for spray combustion

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Liquid spray combustion plays an important role in many practical devices, such as aircraft engines, liquid rocket and internal combustion motors. The understand-

ing of such flames is of key importance for design and optimization of such devices, especially given the complex and multi-disciplinary phenomena involved. To mention a few, the occurrence of preferential evaporation effects due to different volatiles of multi-component realistic fuels and the simultaneous existence of multiple combustion regimes. In order to singularly analyze these effects, canonical configurations of spray flames are commonly employed. In particular, counterflow spray flames have been widely employed using different strategies to inject fuel droplets. Parametric analysis have then been performed based on droplet diameter, global equivalence ratio or strain rate, in order to asses their effect on the ensuing flame structure.

In this work we present a numerical framework coupling multi-component evaporation with a finite-rate chemistry solver. The mentioned framework is applied to the simulation of a paradigmatic counterflow flame configuration to investigate preferential evaporation and combustion characteristics on realistic aviation fuels.

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Numerical simulation of heat transfer and evaporation of a sessile droplet on a hot wall

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A good understanding of the heat transfer mechanism between impinging spray and the combustion chamber wall in compression ignition engines is needed to reduce the heat loss through the wall and improve their thermal efficiencies. This study investigates the effect of the wall wettability on the heat transfer and evaporation of a sessile droplet on a hot wall in a uniform flow by applying three-dimensional numerical simulations accounting for evaporation from the gas-liquid interface. The wettability is considered by applying a contact angle based on height function methodology. The gas-liquid interface is captured using the volume of fluid method. The results show that after a droplet passes over the wall, the wall is cooled under all wettability conditions. Additionally, the droplet is heated by the heat transfer from the wall and cooled on the windward side due to the latent heat of evaporation which is active there. Furthermore, decreasing wettability enhances the formation of the circulating flow inside the droplet, which significantly affects the temperature distribution there and the wall heat transfer characteristics.

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Mechanism of the trans-critical phase change process for binary methanol-heptane droplets

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The trans-critical transition process of fluids refers to its thermodynamic trajectory from the sub-critical state to the supercritical state. In current study, the trans-critical phase change of binary alkane-methanol droplets is investigated by the molecular dynamic methods in different ambient temperature and pressures, and in different blending ratios of the blends. Using a new approach from the perspective of analyzing the atomic pair entropy fingerprints, we quantitatively distinguish different stages in the trans-critical process of binary alkane-methanol droplets based on the degree of fuel molecular disorder within the fluids near the droplet surface, and identify the transition of phase-change from the subcritical-like evaporation mode to the supercritical-like diffusion-dominated mode. It is discovered that the azeotropy and preferential evaporation phenomena are inhibited at high ambient pressures. The findings also indicate that with the increasing proportion of methanol in the binary droplets, the phase change mode tends to show more subcritical-like feature owing to the introduction of higher critical pressure and hydrogen bonding effect. Finally, the influence of ambient temperatures and pressures on the mode transition of trans-critical phase change is discussed systematically.

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Track07-2 Droplets and sprays (2)

Chair: Jiangkuan Xing
Wednesday, May 8; 13:30 - 14:50; Room C

Turbulent spray combustion modelling based on similarity mapping

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For the purpose of design and application, reliable predictions of turbulent spray combustion are of particular importance. However, there are modelling challenges which are still not well resolved, e.g. coupling between liquid vaporization and chemical reaction. Recently, a similarity mapping approach has been developed and implemented to case tests. With some reasonable sim-

plification, the two phase governing equations can be reformulated as equations in the single gas phase with reconstructed spray-related source terms. Solutions in a laminar counterflow configuration assume interesting similarity features, such as the (almost) independence of the evaporation path after mapping onto a newly defined quantity R, constructed from sensible enthalpy and mixture fraction. In this regard, the flamelet tabulation dimensionality can be hopefully reduced, which then provides a different scenario to understand the spray combustion physics. Upon the conventional flamelet/progress variable model, the flamelet library is constructed from a series of quasi one-dimensional spray counterflow solutions, integrated with the multiple solution modes. Test cases, including the laminar spray counterflow flame and Sydney spray turbulent flame, indicate that this newly proposed model is in principle favorable to improve the numerical predictability with acceptable computational cost.

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Large eddy simulation of a swirling spray flame using the two-phase spray flamelet model

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Turbulent spray combustion widely exists in a variety of energy power systems, and the strong turbulence-chemistry interactions (TCI) lead to the demand for accurate combustion models. Our recently developed two-phase spray flamelet/ progress variable (TSFPV) model has shown sound performance in spray combustion modeling because it can consider the effect of droplet evaporation on the flamelet structure. The previous validation of the TSFPV model focused on simple configurations of non-swirling jet spray flames. In this work, the TSFPV model is further applied to the complicated configuration of the Cambridge swirling spray flame. The M-shaped flame is correctly reproduced by comparing the contour plots with experimental images. Quantitative statistics of the liquid phase achieve a good agreement with the experimental measurements in terms of droplet diameters and velocities. The complex flame structure is further analyzed, with an emphasis on the inner flame in the two-phase spray combustion regime. Some droplets penetrate the flame and the evaporation source term cannot be ignored in the flame region, representing the significant droplets/ flame interactions. Scatter plots of droplet axial velocity illustrate the droplet dynamics with different sizes. The droplets with smaller diameters achieve a velocity balance with the surrounding gas, while the larger droplets penetrate the inner recirculation zone (IRZ) and the inner flame zone. In conclusion, the TSFPV model is well-validated on the Cambridge swirl burner, and the flame analyses deepen the understanding of the two-phase spray flame structure.

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Combustion of Suspended Droplets in Normal Gravity Conditions

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In the last few years, several models for the simulation of phase change using multiphase CFD have been proposed. Most of these models assume constant physical properties, which limits their applicability to benchmark phase change simulations. In this work, we extend a VOF-based phase change model to simulate combustion of realistic droplets, suspended on a solid fiber in normal gravity conditions. This configuration has been widely studied in experimental works, but no numerical models that are able to combine: i) interface-resolved evaporation; ii) suspension by the action of the surface tension force; iii) variable physical properties; iv) combustion chemistry, have been proposed. This work combines these features resulting in a generic model which describes the combustion of multidimensional droplets, including buoyancy effects, thermal expansion, and complex kinetics. The results obtained using this model are in good agreement with experimental data, and they reveal interesting flow features that cannot be resolved using more widespread spherically symmetric models. The implementation is based on the Basilisk code; the code and the simulation setup are freely available on the Basilisk sandbox.

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Analysis of Evaporation Rate in Detonation Induced Break-Up of a Droplet

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Detonation based propulsion has the potential to achieve improved performance as well as offering a smaller lighter combustors. There is particular interest in using denotative propulsion for hypersonic applications due to the rapid rate of combustion within a detonation allowing for shorter combustors and lower inlet compression. Practical detonative propulsion systems will

utilize liquid fuels resulting in a detonation propagating through a mist of liquid droplets. It is currently unknown if the detonation can break-up and evaporate in time to support the detonation directly. To better understand this process high fidelity simulations of a droplet being struck by a detonation wave will be performed and the break-up and evaporation of the droplet will be investigated. These studies will be conducted using an diffuse interface approach with thermo-chemical relaxation to capture the evaporation and cavitation. The analysis will focus on the droplet evaporation rate to better estimate the amount of vapor released near the detonation compared to evaporation after the detonation passes. This will provide insight into how liquid fueled detonation engines operate and the percentage of mass consumed by the passing detonation and fuel vapor remaining behind the detonation.

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Track07-3 Droplets and sprays (3)

Chair: Junji Shinjo
Wednesday, May 8; 15:30 - 16:50; Room C

A Computational Simulation Method for Spray Flows with a Generalized Primary Atomization Module

Jungeun Park, **T.-W. Lee**
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In prior works, we have developed an analytical framework based on integral form of the conservation equations, which leads to an expression for the Sauter mean diameter as a function of the injection and fluid parameters. This has been validated for a range of injection geometries. Since this analysis works for control volumes drawn from the injector exit to any points in the flow field, it can be adapted in a computational fluid dynamic (CFD) framework. CFD is quite effective in determining the continuous liquid velocity field and also discrete droplet motion, but becomes very costly at the droplet formation scales due to high spatial and temporal resolutions required. Thus, the primary atomization process can be boxed into the control volume analysis, and linked as the drop size calculation algorithm, along with a strain-rate Weber number. These aspects of the computational procedure will be discussed, along with application examples in some injection geometries such as pressure-atomized sprays, liquid jets in cross flow, and flat spray nozzle flows.

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Numerical comparison of single- and multi-hole marine-sized injectors

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Present work provides a comparison of the reacting performance of a single- and a multi-hole diesel injector in a marine-sized constant volume chamber using tabulated combustion model and RANS framework in OpenFOAM. Given the dimensions involved, both in terms of nozzle (~1mm) and chamber diameter (500mm), a tabulated combustion model such as the Flamelet Generated Manifold is a convenient choice to keep the computational time low with reliable results. After validating the mesh in terms of liquid length and spray penetration, the reacting cases are compared with experimental results in terms of Ignition Delay Time (IDT), Lift-Off Length (LOL) and Ignition Location (IL), both in single- and multi-nozzle configuration. Moreover, the performance of a two-equation soot model is tested in the multi-nozzle configuration, where recent experiments provided new insights in the emission production. Then, given the amount of fuel injected with large and multiple nozzles, the effectiveness of the specific enthalpy as an additional control variable for the FGM manifold in capturing the heat exchange, without phase changing, between droplets and surrounding gas is assessed.

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Numerical Modelling of Liquid Ammonia Injection

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Ammonia is one of the major candidates as an energy vector of the future because of several characteristics that facilitate its operation, such as the absence of carbon emissions associated with its combustion. Ammonia is generally vaporized before utilization, but liquid injection is an attractive alternative. Liquid ammonia experiences flash boiling when depressurized upon entering the combustion chamber. Numerical modelling of liquid ammonia atomization is a formidable task given the complexity of phase change and atomization co-occurring. One of the main challenges consists of predicting and eventually quantifying the occurrence of nucleation.

The method proposed in this work consists of adopting a phase-field approach to model phase change without relying on sub-models. The model is based on an extension of the nonconvex bulk Helmholtz free energy accounting for interfacial energy following the Van der

Waals theory of liquid-vapour phase change. The physical description ultimately requires the solution of the non-isothermal Navier-Stokes-Korteweg equations.

The system of PDEs was solved by adding a relaxation term to the equation with the scope to make it hyperbolic.

The numerical model was validated against benchmark cases before being applied to ammonia injection. Spontaneous nucleation was observed in the case tested.

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Track09 Heterogeneous combustion

Track09-1 Heterogeneous combustion (1)

Chair: TBD
Wednesday, May 8; 10:40 - 12:40; Room L

A PBE-CFD approach for investigating the asymmetric envelope flame around a burning aluminum particle

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In support of our transition towards a sustainable and carbon-free energy economy, metals are currently investigated as potential recyclable energy carriers that can be exothermally burned in air. A major challenge for the recovery of the metal oxide combustion products is the formation of nano-sized oxide smoke fines. Following metal evaporation and gas phase oxidation, oxide smoke droplets nucleate from gaseous precursors and grow by condensation and coagulation. In order to predict the size distribution of the oxide smoke droplets and investigate their propensity to deposit on a burning aluminum particle, we present a comprehensive and kinetically detailed single particle combustion model in which the particle's reactive boundary layer is spatially and temporally resolved. The dynamics of the smoke's size distribution are governed by a population balance equation (PBE) that is solved in conjunction with a reactive flow solver (CFD). Although the model is tailored to the combustion of aluminum, it may readily be adapted also to other metals. A particular novelty of our contribution lies with the incorporation of a time-varying fuel particle morphology, permitting an analysis of how morphological changes influence the shape of the envelope flame and the migration of smoke towards the particle. Following a validation based on experimentally measured burning times and residue sizes, we instrument the model to assess the cumulative pollutant charge emitted from a particle over the course of its lifetime.

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On the limiting mechanism of single iron particle combustion

Leon Thijs, XiaoCheng Mi, Jeroen van Oijen, Philip de Goey
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Iron powder is considered as a promising metal fuel since it is inherently carbon-free, recyclable, compact, cheap and widely available. To design and improve real-world iron-fuel burners, an in-depth understanding of the fundamentals underlying the combustion of single iron particles is required. Since iron burns in a heterogenous way, it was believed that no iron was lost through evaporation during the combustion process. However, our research has demonstrated that, despite the particle temperature remaining below its boiling point, a small but non-negligible mass loss occurs through evaporation. Furthermore, for iron particle combustion, it has been hypothesized that the oxidation rate of an iron droplet is the result of an interplay among three mechanisms: (1) External diffusion of O_2 from the ambient gas to particle surface, (2) surface chemisorption of, and (3) internal transport of Fe and O atoms. In this study, we explore these limiting mechanisms through the utilization of various numerical methodologies, including boundary-layer resolved models, zero-dimensional models, and molecular dynamics simulations.

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Modeling single aluminum particle combustion in various oxidizers

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Aluminum particles exhibit high energy density, making aluminum a promising carbon-free energy carrier for future energy systems. Aluminum can react with various oxidizers, including O2, CO2, and H2O. The combustion of aluminum particles is intricate and challenging to model. In particular, at elevated particle temperatures, solid aluminum may melt into liquid and evaporate, resulting in

a diffusion flame in the surrounding gas. On the particle surface, both evaporation of liquid aluminum and heterogeneous reactions of liquid aluminum with oxidizer may occur, which is not considered in existing models in the literature. In simulations of practical applications involving a large number of particles, resolving the boundary layer around individual particles becomes infeasible. Instead, point particle approximation without resolving the boundary layer is typically employed. This study proposes a single-particle combustion model for the point particle approach, considering simultaneously the evaporation and heterogeneous surface reactions. Simulation results are compared with experiments on single aluminum particle combustion in different oxidizers, covering conditions where heterogeneous surface reactions and evaporation are of various importance. Additionally, the proposed model is compared with existing models in the literature that involve different assumptions and simplifications.

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Carrier-Phase DNS of Metal Particle Combustion in a Turbulent Shear Layer

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A carrier-phase DNS (CP-DNS) of iron particle combustion in a turbulent mixing layer is presented. The upper stream of the mixing layer features iron particles suspended in cold air, while the lower stream provides hot air moving in the opposite direction. All scales of the gas phase are resolved by DNS in the Eulerian framework, while the solid particles are described in the Lagrangian framework. The combustion of iron particles is described by an already existing sub-model implemented in the dispersed phase which interacts with the carrier phase by means of momentum, mass and heat exchange. Additionally, the dispersed phase is considered to be dilute; therefore, no direct particle-to-particle interaction is taken into account. In this work, the previous simulations in this context are cross-validated, extended by focusing on the effect of particle size, and further analysis is presented. This analysis explores the interactions between the gas and particle phases, as well as the effects of turbulent structures on the particle combustion behavior, including ignition time and mode of heterogeneous combustion (kinetic/diffusion limit). Additionally, heat transfer is studied in detail by investigating the effects of radiation and temperature distributions in both phases.

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Track09-2 Heterogeneous combustion (2)

Chair: Kazuki Tainaka
Wednesday, May 8; 13:30 - 15:10; Room L

NOx emissions of iron aerosol flames

Thijs Hazenberg, Catharina E.A.G. van Gool, Jeroen A. van Oijen, Laurentius P.H. de Goey
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In recent years, metal fuels have gained significant attention as an alternative carbon-free energy carrier. Iron is particularly interesting, as the boiling point of iron is above the stoichiometric adiabatic flame temperature, i.e., the products are mostly solid micron-sized particles. While carbon-based emissions (CO, CO2, soot, etc) are not a concern, iron nanoparticles and nitrogen oxides are, because: The combustion occurs below the boiling point of iron, however, a small fraction can evaporate and as high temperatures are involved, nitrogen oxides (NO) are formed. In this presentation, freely propagating iron aerosol flames are utilized to study emissions. In lean iron dust flames, the particle temperature can significantly exceed the adiabatic flame temperature, which raises concerns about NO formation in the boundary layer. Using a posteriori analysis, we show that these boundary layer emissions can be neglected. In the bulk gas phase, the key mechanism of nitrogen oxide emissions is identified. As expected, avoiding high temperatures is useful for the reduction of emissions.

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Flame characteristics of iron dust counter-flow flames

Catharina E.A.G. van Gool, Thijs Hazenberg, Jeroen A. van Oijen, Laurentius P.H. de Goey
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The need for alternative carbon-free energy sources has led to extensive research on metal dust as a fuel. Iron powder in particular has some promising characteristics: the particles do not exceed the boiling temperature of iron(-oxides) upon combustion and (volumetric) energy densities are comparable to those of hydrocarbons. For gaseous flames, it is well understood that flame characteristics can be modified by stretch effects. For iron flames, stretch effects are at least as important. Additional complexity due to the inertia of the particles asks for a new model to describe the particle flow strain. In this

study, iron dust counter-flow flames are utilized to investigate the impact of particle strain on the flame structure. Two major effects are identified: preferential diffusion due to the infinite Lewis number of iron powder, and an inertia effect. The inertia of the particles leads to a particle flow strain lower than the gas flow strain, causing an increase in powder concentration. The extent of this effect is particle size dependent.

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Flame structure and burning velocity of hybrid methane-iron air flames

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The burning velocity of micron-sized iron powder in air is slow; therefore, iron flames are difficult to stabilize in an experimental setup and industrial burners. A support fuel can be used to stabilize iron flames in experiments by enhancing the burning velocity. We performed numerical simulations using methane as a support fuel, as the combustion characteristics of methane burning in air are well known. Numerical simulations are used to investigate the addition of iron powder to methane-air flames, exploring various particle sizes and concentrations while maintaining a constant equivalence ratio of the methane-air mixture. The burning behavior of iron powder is found to be influenced by factors such as particle size, equivalence ratio and concentration. A critical concentration is identified, at which a sudden change in the flame structure is observed. Below this critical concentration, iron particles burned individually without forming a flame front, while above this concentration, a flame front is observed with complete conversion of iron particles. The laminar burning velocities obtained from the simulations are compared to experimental results.

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Reductive Activation of Commercial Iron Ore Materials using H2 and NH3 for Ammonia Synthesis and Decomposition

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The reduction behavior of commercial iron ore materials (Sigma-Aldrich), comprising crystalline Fe2O3 and Fe3O4 along with minor impurities like silicate and aluminate, was studied using temperature-programmed methods with utilization of H2 and NH3 as potential green energy carriers. It revealed that the reduction of iron ore to metallic iron is more efficient in H2 than in NH3. The latter potentially resulted in a mixture of iron (major) and iron nitride (minor). However, both H2- and NH3-reduced iron samples exhibit activity in subsequent NH3 synthesis and decomposition applications, representing typical reactions for the production and extraction of a hydrogen carrier. More importantly, the reduced iron samples show a high ability to entirely decompose NH3 at temperatures below 600 °C and ambient pressure, approaching the performance of conventional Ru catalysts, albeit at a higher cost. This research provides new insights into the production and utilization of green H2, with a particular focus on green NH3, using economically viable, commercially available iron ore materials.

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Track09-3 Heterogeneous combustion (3)

Chair: Oliver Stein
Thursday, May 9; 09:50 - 12:30; Room L

3D CFD particle-resolved simulations of heterogeneous combustion of non-porous char in a fixed-bed reactor

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This work aims to numerically study a 3D chemically reacting fixed-bed for non-porous char under gasification and flow regime conditions. Particle-resolved simulations

were performed using the commercial software Ansys Fluent, implementing a six semi-global kinetic scheme, consisting of carbon monoxide combustion, forward and backward water-gas-shift reaction, Boudouard reaction, and two other heterogeneous reactions. The fixed-bed was composed of 85 spherical particles with a 5.6 mm diameter, located in the bed zone and subsequently placed in a stationary position. Several Reynolds numbers, inflow gas temperatures, and inlet mass fractions of oxygen ($Y_{O2,in}$) were assessed. Experimental tests were conducted to contrast numerical results. Mass fraction of species showed consistency when describing heterogeneous combustion, where the Boudouard reaction and carbon monoxide oxidation were dominant among heterogeneous and homogeneous reactions, respectively. The inflow gas temperature was a critical parameter to assess since the kinetic scheme is notably activated from 1300 K. Moreover, the highest temperature and carbon dioxide concentration difference between particle surface and gaseous phase were 0.39% and 29.70%, respectively. A linear dependency for species concentration and temperature at low $Y_{O2,in}$ was observed. This study may be considered as a benchmark case for validation of 1D and 2D models.

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Numerical study of the mechanisms of convective burning of black powder

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The work addresses the clarification of the mechanisms of convective burning of an extended black powder charge. The hyperbolic Baer-Nunziato-type model is used. Although the Baer-Nunziato equations have been used for the simulations of combustion and detonation of heterogeneous explosives for a long time, there are only a few works in which this model is used for gun powders. The model takes into account the compaction effects of the gun powder as well as mass, momentum, and energy interphase exchange between powder and gas. The numerical algorithm is based on the Harten-Lax-van Leer or Godunov method with the pressure relaxation procedure. Intergranular stresses in the phase of particles are taken into account. The statement of the problem corresponds to the full-scale experiment of B.S. Ermolaev with co-authors (Semenov Institute of Chemical Physics of RAS). The correct wave pattern is obtained in the simulations, namely, the leading compaction wave, the combustion wave that follows the previous one, and the waves reflected from the side walls of the channel at the latter stages of the process. The explanation of the pressure curves at the transducers along the channel is given. The comparison of the simulation results with the experimental data and simulations of B.S. Ermolaev is carried out.

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Heterogeneous Combustion of AP/HTPB/RDX Propellants with Detailed Kinetics

Pierre Bernigaud[1], Dmitry Davidenko[1], Laurent Catoire[2]
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Composite solid propellants include as main constituents a binder, producing combustible gases by its pyrolysis, and particulate components, which generate oxidizing gases. Ammonium perchlorate (AP) is a widely used ingredient for solid propellants, together with a polymeric binder such as the hydroxyl-terminated polybutadiene (HTPB). These so-called AP/HTPB composite propellants have been extensively studied in the past. Next-generation propellants may include nitramine (RDX or HMX) particles as a partial replacement for AP for some specific purposes.

This study proposes a detailed kinetic model for the combustion of the AP/HTPB/RDX ternary system. It is shown that the model reproduces the main combustion characteristics of the studied ingredients. The reactions mechanisms for the considered materials have been validated with respect to fundamental experiments.

Employing this combustion model, a flame above an AP/HTPB/RDX composite propellant is simulated. The considered 2D axisymmetric configuration represents an RDX particle surrounded by a homogenized binder composed of fine AP particles and HTPB. To the authors' knowledge, this is the first simulation of such a flame in the literature. A study on the effect of pressure and RDX particle diameter is conducted. It is shown that for each RDX particle size, a pressure limit exists, below which the RDX particle combustion becomes slow with a flame typical for the so-called dark zone, . Reducing the RDX particle diameter hence decreases the overall regression rate. This behaviour is opposed to the one observed with conventional AP/HTPB propellants.

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Numerical approach to understand factors affecting catalytic decomposition of methane

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As the world looks for cleaner and more sustainable energy, there's a growing need to find better ways to produce hydrogen. Turquoise hydrogen, made by mixing methane in a special way that captures carbon emissions, is a better way to make hydrogen without adding more carbon to the atmosphere.

This research employs Computational Fluid Dynamics (CFD) simulations to scrutinize and enhance the turquoise hydrogen production process. The simulation model is intricately designed to capture the reactor system's fluid dynamics and chemical reactions during turquoise hydrogen production. The model's geometry incorporates a porous cylindrical region and a fluidized bed reactor, with the domain extending at the top and bottom to observe reactions and catalyst deactivation. The catalyst employed in this study is Ni-Al2O3.

To optimize production efficiency, the model is simulated under various inlet conditions, specifically different mass flow rates of methane (20, 50, and 100 ml/min) and different concentrations of catalyst viz 65 wt.% Ni-Al2O3, 90 wt.% Ni-Al2O3 at varying wall temperatures (550, 650, and 700 degrees Celsius). Additionally, the model undergoes simulations at different operating pressures, ranging from 1 to 5 bar. The CFD simulations comprehensively consider heat, mass, and momentum transport phenomena, coupled with detailed reaction kinetics. This approach provides a thorough understanding of the intricate interactions within the system, contributing to optimizing turquoise hydrogen production.

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Parametric study on optimal operation of burning-off process for the removal of deposited carbon in a coke oven

Keh-Chin Chang, Yi-Da Chung
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Removal of deposited carbon in coke oven is a regular task in the coking-making operation, either by traditional manual removal during maintenance downtime or by burning them off with air injected through the charging holes before recharging coal into the coke oven. Numerical study for the burning-off carbon deposits with air-injection process exists in literature but not many. The chemical reactions that are involved in the burning carbon deposits include heterogeneous and homogeneous reactions over the heated wall surfaces in oven. It was noticed that the first near-wall grids in the computational mesh should be placed within the viscous sublayer of the wall boundary layer for accurate calculation of the heterogeneous reaction rate. A typical coke-oven battery is composed of the oven chamber with an ascension pipe and four coal charging holes at the top of the chamber. Carbon deposits generally accumulate on the upper side walls and the rooftop of the chamber and the goosenecks of the charging holes. A series of parametric study on the operational conditions, including which charging hole with how much air injection rate and how deep the air blowing lance should be inserted into the chamber, will be conducted using a developed numerical model to search for the optimal operation in question.

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A priori analysis on an extended flamelet/ progress variable model for coal/ ammonia co-firing flame

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Ammonia/coal co-firing is considered a promising technology for reducing CO2 emissions, but the presence of multiple fuel streams and nitrogen sources makes accurate and efficient modeling of combustion and NO formation challenging. In this study, a point-particle direct numerical simulation (PP-DNS) work with detailed chemistry for coal/ammonia co-firing flame was carried out, and an extended flamelet/progress variable was developed to account for the multiple fuel streams and reacting stages. The extended model was then evaluated through a priori analyses with the PP-DNS solution as benchmarks to assess its performance, demonstrating its capability to accurately replicate the gas temperature, major species, and CO profiles derived from DNS. The formation of NO occurs with the same-order time scale as that of the major species in this flame, allowing for acceptable prediction by directly extracting data from the flamelet tables. Interestingly, including NO in the progress variable did not improve the prediction for NO and instead decreased the accuracy of temperature and major species predictions. The main deviations of NO prediction can be attributed to ignoring the multi-dimensional effect.

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Numerical Analysis of MILD Combustion of Pulverized Biomass-Coal Flame

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Combustion continues to play an important role in the area of renewable energies. Besides the role of hydrogen, this is due to the role of biomass, which is increasingly attracting the attention of researchers. For high thermal powers, where solid fuels are burnt in pulverized form, biomass is quite often fired in combination with the fossil fuel, coal, i.e. in the co-firing mode, which is the subject of the present work.

MILD combustion is considered as a promising combustion mode due to its advantages of cleanliness and high efficiency. It has a wide range of fuel flexibility and can remarkably diminish the NO emissions. In pulverized biomass-coal co-firing, the combustion is likely to be driven by biomass, due to its comparably higher volatility and ignition characteristics. The ignition time and mode of biomass and pulverized coal are different like their burnout times, as the faster burning biomass can "rob" oxygen from coal. These interactions have not yet exhaustively explored for MILD pulverized co-firing of biomass and coal.

For throwing more light onto the above-mentioned issues, experiments were performed by Fu et al. [1-3] in a pilot-scale furnace, quite recently.

In the present work, the MILD pulverized biomass-coal flames measured by Fu et al. [1-3] are numerically analysed, to assess the prediction capability of different computational approaches and mathematical models for this type of combustion. In general, there is a rather high uncertainty in the pyrolysis rate of biomass. Applying different suggestions, the effect of this uncertainty on the results is assessed. Beyond model validation, the complex processes of MILD co-firing will be analysed.

[1] Hu, F. et al. Energy & Fuels 2019, 33, 12791-12800.
[2] Hu, F. et al.. Fuel Proc. Techn. 2022, 230, 107222.
[3] Hu, F. et al. Fuel 2023, 342, 127768.

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Track10 Detonation, explosions

Track10-1 Detonation, explosions (1)

Chair: Hiroshi Terashima
Wednesday, May 8; 13:30 - 15:10; Room B

Large Eddy Simulation of Rotating Detonation Rocket Engines at Three Operating Conditions

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In this study we examine three high-fidelity large eddy simulation of rotating detonation rocket engines to understand how to quantify the performance of the device from simulation data. The nature of the rotating detonation engine makes geometric simplification difficult, as a result the full 360-degree geometry must be included in the simulation. This large simulation domain greatly increases the simulation cost. Simulations are run using an in-house finite volume CFD solver with finite rate chemistry. A novel grid stitching system is used to build-up the complex geometry in the multi-block framework. This framework allows different non-conformal meshes to be joined together to construct the large geometry. Three different operating conditions are simulated to examine the effect of mass flow rate and overall equivalence ratio has on the devices behavior. The results show that the mass flow rate has a strong effect on the operating pressure and strength of the detonation waves observed inside the chamber. To elucidate the behavior, a number of post-processing techniques have been developed to better understand the dynamics inside the engine. These include the ability to separate how much of the combustion is tightly coupled with the detonation mode and how much is instead deflagration. These tools will be used to quantify the performance of the device at the different operating points.

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Numerical Analysis of Exhaust Jet Characteristics from Annular RDEs with Various Outlet Geometries

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The behavior of exhaust gases from the outlet of the annular rotating detonation engine (RDE) with which the outlet geometry is changed and the interference with supersonic airflow were investigated to examine the feasibility of operating a traditional rocket type RDE in a rocket-air breathing hybrid mode. The analysis was performed on an annular RDE with its outer wall curved into several shapes, and on the area downstream of the combustor outlet. The mainstream air was regarded as supersonic air flowing into a combustor, and the propellant for the RDE was premixed hydrogen-air gases under fuel-rich condition. As a result, the different behavior of the exhaust jet was observed compared to that of the case using an RDE with a normal outer wall shape. The mixing with supersonic airflow was also confirmed when it was considered to flowing outside the RDE, which indicating that altering the outer wall geometry of the combustor is one of the effective way for operating an orthodox rocket mode annular RDE in the air breathing mode. At last, comparison of the thrust of the combustor in rocket mode and hybrid mode operations was considered.

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The mechanism of a resonant amplification of pulsations behind a detonation wave propagating in a non-uniform mixture

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Propagation of detonation waves in non-uniform gaseous mixtures has become a matter of interest over the past several years due to the development of rotating detonation engines. We developed an algorithm for the simulation of detonation propagation in a non-uniform

medium in a shock-attached frame of reference. One-dimensional reactive Euler equations with single-step Arrhenius kinetics were solved. Using the developed algorithm, a numerical study of the propagation of a stable detonation in a medium with variable density was carried out. We carried out a series of simulations, varying the wavelength of the disturbances. As a result, several different modes of pulsations of the detonation wave speed were obtained. We got a nonlinear dependence of the amplitude of these pulsations on the wavelength of disturbances with resonant amplification of pulsations for a certain range of wavelengths. The effect is explained using the characteristic analysis in the x-t diagram.

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Simulation of Pulsating and Cellular Detonation in Gases with Small Heat Release

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We consider the nature of both pulsating and cellular detonation in gases modeled with a one-step Arrhenius chemical reaction for small heat release. With the one-step model, regimes of stable two-dimensional detonations can be found for small activation energies provided the heat release remains moderate. As the activation energy is increased, the magnitude of the heat release required for stable two-dimensional flow decreases rapidly. For large activation energies only very small amounts of heat release generate stable two-dimensional flow. Moreover, only small increments in heat release are needed to drive the flow first above the neutral stability boundary for two-dimensional cellular instability, and then above the stability boundary for one-dimensional pulsating flow. We examine, numerically, the structure of pulsating and cellular Chapman-Jouguet detonation in gases with small heat release using an inviscid, reactive Euler equations framework. Due to the small amounts of heat release, such simulations required careful treatment of numerical dissipative effects. Additionally, we use a shock-fitted, shock-attached frame that treats the detonation shock as a leading boundary of the flow.

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Numerical simulation of detonation initiation over obstacles using the AMReX library

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In this research detailed detonation analysis supports complex geometries, and can be calculated using a supercomputer. In particular, the Adaptive Mesh Refinement (AMR) and Embedded Boundary (EB) methods provided by the AMReX library are expected to make a significant contribution to the generation of complex geometries required in detonation analysis and to the reduction of calculation costs. In addition, the MACKS method adopted in the chemical reaction calculations can significantly reduce the computational cost and provide more accurate calculations than the conventional methods. The aim of this study is focused on the validation of the developed CFD code and the confirmation of the effectiveness of the AMR and EB methods for detonation analysis. The initial validation was carried out for the shock tube problem and now we compare numerical analysis with experimental results. In detonation analysis, AMR can contribute to efficient and detailed detonation analysis due to the different mesh resolutions required for the detonation, flame, unburnt, and obstacle areas.

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Track10-2 Detonation, explosions (2)

Chair: TBD
Wednesday, May 8; 15:30 - 17:10; Room B

A detailed numerical investigation of the detonation-bow shock interaction

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The interaction of a detonation with the bow shock generated by objects moving at supersonic speeds has applications in the fields of industrial safety and in the transportation, storage of gaseous fuels such as hydrogen and natural gas. Numerical simulations and investigations into accidents causing vapor cloud explosions (VCEs) have shown that obstacles such as process equipment or other debris can accelerate flames and result in transition to detonation, causing huge economic and material losses. Preliminary investigations of the interaction (ASV and ESO, SciTech 2023) showed that detonation diffraction into the

wake of the object weakens the cellular structure. Analysis of the vorticity budgets (ASV and ESO, 13th USNCM 2023) showed that the baroclinic term and the flow divergence term were important in the diffraction. Here, we perform a detailed investigation of the interaction using two-dimensional reacting and non-reacting numerical simulations. The speed, characteristic size of the obstacle are varied and the interaction with a nonreacting shock, ZND detonation, and a cellular detonation are studied. The compressible flow phenomena such as shock-shock, shock-flame interactions, detonation diffraction, shock-vortex, and flame-vortex interactions are studied by looking at the changes in the state variables and their contribution to the vorticity budget terms. We intend to quantify the effects of combustion heat release and the transverse wave structure on the vorticity budget terms. This investigation is expected to guide full three-dimensional studies of the interaction in the future.

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Numerical simulation of detonation onset from H2-air flame-shock interaction

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The interaction between a flame and a shock is examined in a numerical set-up representative of an experimental set-up based on a centimetric shock tube. A mixture of hydrogen and air at an equivalence ratio of 0.8 is first ignited at the end of the tube which leads to the development of a finger-glove flame toward which a shock is then sent. Realistic mechanisms for the chemistry are employed along with an accurate description of the diffusion including the Soret effect. Gravity is also included. The wall temperature is fixed at 300 K which might appear as a very stringent condition but is better justified than adiabatic condition. The impact of the description of the geometry (1D, 2D, and 3D) on the apparition of a transition to detonation is studied for two values of the incident shock Mach number. Depending on this Mach number, two different types of DDT are observed: one related to shock focusing occurring close to the axis of symmetry of the tube and a second type occurring in the vicinity of the reactive boundary layer. A comparison with experimental results confirms the capacity of the numerical simulation to capture the details of the flame/shock interaction and the necessity of a 3D realistic geometry.

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The structure of triple shock reflections using the 10-moment method

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The structure of a triple-shock configuration and its reflection, characteristic of the cellular structure of detonations, is solved numerically in two dimensions using the 10-moment maximum-entropy model of gas dynamics for diatomic gases. The results are compared to the analoguous problem of single shock reflections on a ramp, demonstrating the equivalence between the two problems. This study demonstrates the potential of maximum-entropy based moment closures as an accurate alternative to traditional hydrodynamic models. The 10-moment model, derived from gas-kinetic theory, is the second member of the maximum-entropy moment closure hierarchy. These moment models are based on an assumed form of the distribution function describing the phase-space probability distribution of gas particles. The 10-moment model for diatomic gas yields a set of eleven hyperbolic first-order balance laws capable of predicting adiabatic viscous flow in both the continuum and rarefied regimes. Its first-order nature provides numerical advantages such as a decreased sensitivity to mesh quality and irregularities. The requirement for the evaluation of only first derivatives also offers the possibility for an extra order of spacial accuracy for a given stencil. The source term used to model the inter-particle collisions is the BGK relaxation-time collision operator. All calculations are computed using a discontinuous-Galerkin-Hancock scheme ensuring third-order accuracy in both space and time. The simulations are run in parallel using adaptive mesh refinement to accurately capture the solutions' structure.

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A molecular view of shocks and triple points: implication on gas-phase detonations

Amitesh S Jayaraman, Ethan S Genter, Hai Wang
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Hydrodynamics around triple point collisions are central to detonation cellular structure. From direct numerical simulations, it has been observed that the vorticity generated at triple points and transported to behind the Mach stem produces a high-speed jet that drives the Mach stem. Although computational fluid dynamics shed light on the dynamics within detonation cells, high-resolution

simulations show that the vortex generation occurs at length scales that can be comparable to the shock thickness, and hence approaches the realm of the molecular scale. In this work, we undertake a molecular dynamics study of the shock and triple point regions of a nitrogen shock that undergoes Mach reflection off a wedge. We observe a region of collision enhancement ahead of the shock and a 'hotspot' in the triple point region, and assess their implications on gas dynamics and chemical kinetics. Furthermore, we investigate the generation of vorticity near the triple point region. The results of this study provide a better understanding of triple point structure that is useful to numerical simulations of detonations.

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Shocks in n-dodecane/nitrogen mixtures: a molecular dynamics study

Ethan Samuel Genter, Amitesh Sivaraman Jayaraman, Hai Wang
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Understanding the transport of long-chain hydrocarbons through shocks is relevant to spray detonation. Shock interaction with aerosolized hydrocarbons in a diluent determines the ignition characteristics of the detonation, and by extension, the structure and stability of the wave. The current study uses molecular dynamics simulations to investigate the molecular transport of n-dodecane in a N2 shock. The large temperature and density gradients within the shock give rise to a thermophoretic and pycnophoretic force, respectively, on the n-dodecane molecules that could preferentially concentrate them ahead of the shock front. Furthermore, n-dodecane molecules also tend to align in the direction of convective flow within the shock, thereby perturbing the molecular diffusivity, and such diffusivity can be anisotropic. We observe the phoretic transport and flow alignment in n-dodecane molecules over a range of pre-shock gas conditions and shock strengths.

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Track10-3 Detonation, explosions (3)

Chair: Pascale Domingo
Friday, May 10; 09:50 - 11:50; Room B

Numerical simulations of the run-up distance to detonation in hydrogen-methane blends

Milin Martin, Elaine S Oran, Ashwath Sethu Venkataraman
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In this presentation, we show selected results from using the multidimensional reactive Navier-Stokes equations (RNSE) to simulate Deflagration-to-Detonation (DDT) in an obstacle-laden channel filled with stoichiometric hydrogen-methane fuel blends in air initially at atmospheric conditions. The new AMRFCT code is used to solve the RNSE using the fourth-order Flux-Corrected Transport (FCT) algorithm with appropriate source terms on an adaptively refined Cartesian mesh. New multifuel Chemical-Diffusive Models (CDMs) are used in the RNSE to represent the chemical reactions leading to conversion from fuel to product, related heat release, and physical diffusion processes. Each new CDM generates an optimized set of parameters that, when inserted in the RNSE, reproduce critical flame and detonation properties of a particular hydrogen-methane blend in air. We discuss how these parameters are obtained for different blends. Of particular interest here is a comparison of the run-up distance to detonation of these mixtures ranging from pure hydrogen in air to pure methane in air.

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Revisiting the issue of deflagration-to-detonation transition in an unconfined system via highly-resolved 2D axisymmetric simulations

Kazuya Iwata, Sho Wada, Ryoichi Kurose
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In most previous studies on deflagration-to-detonation transition (DDT), a wall-confined system has been primarily considered since the reflected shocks and boundary layer take substantial roles in accelerating flame to the Chapman-Jouguet deflagration as the pre-initiation stage. Discussion on DDT in an unconfined system has not reached a consensus yet with only a few relatively weaker experimental evidences. Even though there are few

continuing efforts to evaluate its possibility, it is widely believed that DDT in an unconfined system is not feasible, regardless of strong evidence such as Type Ia supernovae, whose observational outcomes are explained well by DDT in unconfined media.

The authors perform 2D axisymmetric simulations fully resolving the flame structure of unconfined H2/O2 mixtures. Equivalence ratios of premixed H2/O2 mixtures are chosen to be 0.5 and 0.8 to reproduce the conditions explored by Kiverin et al. 2022 and Zel'dovich et al. 1947, respectively. Flame acceleration to Mach numbers of 0.3-0.35 at the radius of 2 cm, where the DDT was demonstrated in Zel'dovich et al. 1947, is observed in both equivalence ratios, but DDT is never evidenced, whereas rougher-resolution studies succeed in DDT and direct initiation. These results pose a challenge to previous numerical studies where rougher resolutions were applied. The effects of the intrusive ignition method in Zel'dovich et al. 1947 should be quantified in the future. Three-dimensional resolved simulations are also being planned to capture the flame dynamics quantitatively by applying an adaptive mesh refinement (AMR) technique.

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Transition from autoignitive reaction wave to detonation under transonic conditions for methane mixture

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A one-dimensional system where unburned premixed gas enters from the inlet boundary and burned gas exits from the outlet boundary is considered. A steady-state solution is obtained when the inlet velocity is equal to the laminar burning velocity under subsonic conditions or equal to the Chapman-Jouguet detonation velocity under supersonic conditions. However, other steady-state solutions could exist, especially if auto-ignition occurs in the system as the inlet temperature increases. Such a reaction waves, which stand at positions where residence times are very close to ignition delay times, are termed as "autoignitive reaction wave." While "autoignitive reaction wave" can be obtained as steady-state solutions over a wide range of inlet velocity conditions under high inlet temperatures in the subsonic regime, it is not clear what solutions can be obtained around the transonic regime. In this study, 1D transient reactive flow simulations were performed for three inlet velocity conditions such as two subsonic and one transonic conditions using methane fuel. As a result, the detonation transition was confirmed when the spontaneous ignition front speed (inverse of the spatial gradient of ignition delay time) exceeded the speed of sound. This suggests that the detonation transition boundary of "autoignitive reaction wave" is determined not only by the shock transition in the transonic regime but also by the relationship between the spontaneous ignition front speed and the sound speed.

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Semi-Confined Reaction Zone Effects in Gaseous Detonations

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Motivated by rotating detonation engines (or RDEs), we consider a continuous detonation in a channel geometry wherein the ambient state has two distinct zones: (1) a region of fresh reactant gases below some standoff distance from the bottom of the channel, and (2) a region of inert product gases above the standoff distance. The resulting flow is characterized by a detonation front connected to an oblique shock, with a shear layer acting as partial confiner between the reacting flow and post-shock product gases. In this work, we will utilize a novel shock-fitted, shock-attached frame to isolate and analyze this system by treating the detonation front and oblique shock as boundary condition of the flow field. Streamline reflection and outflow conditions are utilized for the other boundaries as needed. This work expands upon our previous studies by introducing an ambient state with two distinct regions, thus allowing us to directly simulate the shear layer between the two flow regions. With this implementation, we will assess the effect of standoff distance and confinement via the shear layer with regard to the detonation propagation and stability.

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Detailed Numerical Simulations of Explosive Post-Detonation Afterburning

Ryan Houim, Anthony Egeln
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Numerical simulations were performed in 3D Cartesian coordinates to examine the post-detonation processes produced by the detonation of hemispherical explosive charges in air. The explosive charges considered were PETN, which is nearly soot free, and TNT, which is very sooty. The simulations captured air dissociation by the Mach 20+ shock, chemical equilibration, afterburning using finite-rate chemical kinetics with a detailed chemical reaction mechanism. Soot was modeled using an Euleri-

an multiphase that considered combustion, sublimation, agglomeration, and thermal radiation. The Becker-Kistiakowsky-Wilson real-gas equation of state was used for the gas-phase. A simplified programmed burn model was used to seamlessly couple the detonation propagation through the explosive charge to the post-detonation reaction processes inside the fireball. The computed blast, shock structures, and chemical composition within the fireball agree with literature and companion experimental measurements. The evolution of the flow at early times is shown to be gas dynamic driven. At later times, the Rayleigh-Taylor and Richtmeyer-Meshkov instabilities promote mixing and produce a non-premixed turbulent fireball between the fuel-rich detonation products and shock-heated air. A mixing layer and Damkohler number analysis study revealed that the afterburning processes of small bench-top scale charges is in a finite-rate reaction regime while larger charges transition to a mixing-limited regime. These results indicate that afterburning experiments utilizing small bench-top scale charges need to be used with caution when scaling to larger-sized charges.

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Track10-4 Detonation, explosions (4)

Chair: Kazuya Iwata
Friday, May 10; 13:00 - 15:00; Room E

Continuum Modeling of Steady 1-D and 2-D Detonation Wave Propagation in Porous High Explosives

Joshua Garno, Mark Short, Carlos Chiquete, Stephen Voelkel
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Structural irregularity in high explosive (HE) molding powders results in granular resistance to compaction during pressing. Consequently, pressed HE contains residual porosity which typically occupies about 1-3% of the HE volume. Thermal and mechanical damage can also lead to significant additional porosity in HE materials. It is well-known that HE detonation performance properties are sensitive to the initial HE density, or equivalently, initial porosity. However, the driving physical mechanisms through which porosity affects HE detonation phenomena have yet to be described or modeled in detail. In this work, a continuum modeling approach is used to examine the mechanisms by which porosity affects steady detonation wave propagation in initially porous HEs. Finite-rate compaction of the porous HE material is captured with an evolution equation for the solid volume fraction. The initial porosity and compaction viscosity of the HE are varied to explore their effects on steady 1-D and 2-D detonation wave propagation. Results of 2-D flow computations, performed in an axisymmetric, shock-attached, moving frame of reference, are compiled to produce size effect curves parameterized by the initial HE porosity and compaction viscosity.

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Dynamics of Jet-Stabilized Detonation Waves

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Supersonic jets play an important role in a wide range of aerospace systems. The structure and behavior of inert supersonic jets, both over- and under-expanded, has been studied extensively over the years theoretically and experimentally. At the same time, reacting supersonic jets have received far less attention. Under the appropriate conditions, ignition can occur behind the Mach disk of a highly under-expanded premixed jet, which can result in the formation of a detonation wave. While conclusive experimental observation of such jet-stabilized detonation waves (JSDW) is presently lacking in the literature, several prior numerical studies have suggested the possibility of their existence. At the same time, no comprehensive understanding of JSDW presently exists, including conditions for their formation, as well as their structure and dynamics. Here, we describe a detailed theoretical framework for predicting the conditions of the onset of a JSDW in a 2D slot jet with a single-step Arrhenius kinetics. We also present a large suite of numerical simulations demonstrating the accuracy of this framework and exploring the structure, dynamics, and stability of such JSDW. Finally, we discuss future extensions of this model and its potential relevance both for the fundamental detonation studies and novel propulsion designs.

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Flow characteristics of oblique detonation wave/boundary layer interactions under a hypersonic reactive flow

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Due to the high thermal cycle efficiency and compact combustor, oblique detonation engines hold great promise in the field of hypersonic propulsion. Previous

numerical simulations of oblique detonation waves have predominantly solved the inviscid Euler equations, disregarding the influence of viscosity and boundary layers. However, in real combustion chambers, the interaction between oblique detonation waves and boundary layers significantly alters the flow structure and diminishes engine efficiency. Therefore, this study conducts numerical simulations considering detailed chemical mechanism and the viscosity of the mixture to investigate the interaction between oblique detonation waves and boundary layers within combustion chambers. The results indicate that the wedge-induced oblique detonation wave generates a strong adverse pressure gradient upon impacting the upper wall, leading to boundary layer separation. The separation zone subsequently induces an oblique shock wave near the upper wall. While an increase in wedge angle will cause the transition of oblique shock wave to oblique detonation wave. Besides, the formation of the separation zone reduces the actual flow area within the combustion chamber, leading to a decrease in throat height. When the throat height is small enough, flow chokes, causing the oblique detonation combustion to fail. The polar curve analysis is employed to theoretically explain the formation mechanism of the wave structure under different parameter conditions. The theoretical predictions closely align with the results in simulations. The findings of this study provide new insights into the investigation of the influence of viscosity and boundary layer effects on the structure of oblique detonation waves.

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Detonation Cell Size Prediction with Artificial Neural Networks and Non-Dimensional Features

Georgios Bakalis, Hoi Dick Ng
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In gaseous detonations the cell size λ is commonly used as the characteristic length to quantify the sensitivity of a detonation or to scale different dynamic parameters. In this work we show how this cell size can be predicted using Artificial Neural Network (ANN) models with different number and combination of input features. These models are trained and tested using experimental cell size data for a wide range of reactive mixtures at different initial conditions, combined with the corresponding chemical kinetics parameters, calculated using the steady ZND model. Unlike our previous work, only non-dimensional input features are used, which are created using the ZND parameters. The cell size, which is the ANN prediction target, has also been non-dimensionalized with the induction length (λ/Δi). This approach leads to the development of slightly improved ANN models with a lower mean prediction error (19-23%) compared to the previously developed dimensional ANN models. The predictions of these models appear to be more consistent when different input features are considered, requiring just 2 input features for a good cell size prediction and just 1 for an acceptable one.

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Modulation of the Unstable Cellular Detonation Structure with Microplates

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A detonation commonly exhibits an unstable cellular frontal structure, which affects its propagation and dynamics at critical phenomena. In this numerical work we investigate the modulation of this frontal structure using a series of thin, staggered micro-plates that are embedded in the combustible mixture. Continuing on our previous work, we now take viscous, thermal and momentum diffusion terms into consideration, meaning that the flow is governed by the reactive Navier-Stokes equations, coupled with a two-step induction-reaction Arrhenius chemical kinetics model. The results once again show that a detonation with a regular cellular structure can be obtained from an irregular one that propagates through specific obstacle configurations, without significant velocity deficit. The modulated detonation shows a one-dimensional reaction rate profile that is closer to the ideal ZND, and a burn mechanism mainly by shock compression.

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What controls the cell size in gaseous detonations?

Abeetath Ghosh, Sandeep Dammati, Alexei Poludnenko
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Detonation cell size is one of the central characteristics of a detonation wave due to its empirical correlation with several key detonation properties, including minimum channel size, critical tube diameter, etc. It is unclear if modern multi-dimensional numerical simulations can predict accurately the detonation cell size for practical fuels. Prior studies have reported a discrepancy for hydrogen-air mixtures between the experimental measurements and cell size values computed using complex multi-step kinetics. Here we show that even larger disagreement

exists for a wide range of hydrocarbon fuels, including

methane, acetylene, ethylene, and JP-10. Both the cause of this disagreement, as well as the fundamental mechanisms controlling the cell size, remain unclear. To help address these open questions, here we systemically analyse the effect of activation energy and gas compressibility on the detonation cell size in the context of single-step kinetics. In particular, we explore the cell size dependence on the induction length and thermal width, with the focus on the relative importance of different shock over-drives, which are present in a multi-dimensional detonation front. Finally, we use these results to discuss potential limitations of the existing physicochemical models, which can limit the accuracy of the predicted detonation cell sizes.

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Track10-5 Detonation, explosions (5)

Chair: TBD
Friday, May 10; 15:20 - 17:20; Room E

Influence of SGS combustion models in LES of methane-air deflagration

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Accidental gas explosions in fuel processing industries are devastating. To understand the phenomenon at an industrial scale, investigations are often performed on small-scale geometries that may represent industrial-scale configurations. In this study, a large eddy simulation (LES) of methane-air deflagration in a semi-confined explosion chamber was performed. The chamber includes three obstacles sequentially placed at equal pitch. The sub-grid scale combustion models by Charlette et al. (Combust. Flame, 2002) and Colin et al. (Phys. Fluids, 2000) were implemented and assessed using the XiFoam (a premixed turbulent combustion solver in OpenFOAM). XiFoam uses the flame surface density (FSD) approach to model combustion. The predicted flame speed and the overpressure time history were compared against the experimental data by Patel et al. (Proc. Combust. Inst, 2002). Both models were able to reproduce the flame's accelerating and decelerating behavior across the obstacles. The model of Charlette et al. performs better in predicting the flame speed than the model of Colin et al. Further, the predicted peak overpressure by both models is in close agreement with the experimental data. However, the time of occurrence of the peak is well captured by the model of Charlette et al.

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Numerical Modeling a Polymer-bonded Explosive Frictionally Heated by an Ultrasonic Horn

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We present the numerical modeling of a polymer-bonded explosive which is frictionally heated by an ultrasonic horn. This experiment was conducted by the Dlott-group at the University of Illinois (Men et al., J. Phys. Chem. C, 2018). They observed a two-stage reaction of the explosive: The first stage occurred at the condensed-phase and the second stage was due to the confined reactive gases from the previous condensed-phase combustion. We examine the reaction path of frictionally heated explosives by focusing on the first stage of the reaction. A 0.5 mm length explosive surrounded by an inert polymer subjected to the ultrasonic horn is modeled. The two-component Wide-Ranging equation of states (EOS) is used to model the explosive materials while the Mie-Grüneisen EOS is used for the inert polymer. A harmonic boundary condition is applied to mimic the behavior of the ultrasonic horn in the experiment. The interaction between the explosive and the harmonic waves are mainly discussed.

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DDT as a Hopf bifurcation

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There is evidence that the DDT process may be quite sensitive to apparent details in the kinetic scheme. Overly simple schemes may not be truly meaningful. Complex schemes claim realism, but they may not reproduce experimental detonation results. While stiff integration schemes ensure absolute stability, they do not actually resolve steps too fast to be resolved. Their complexity also may stand in the way of a proper physical interpretation. To gain understanding on the role of kinetics, we consider a range of increasingly complex simplified schemes, up to five steps, with two parallel chemical paths. A one-dimensional simulation follows a methodology relying on experimental flame acceleration data. This allows us to focus upon and resolve the DDT process.

One might expect that when DDT occurs, one eigenvalue of the chemical Jacobian matrix, initially all nega-

tive, becoming positive. For both our three and five step schemes, the independent term in the characteristic equation is positive definite, so that no eigenvalue is ever zero. Instead, a Hopf bifurcation occurs: a complex pair sees its real part go through zero. However, the independent term being small, complex eigenvalues occur over a range so narrow that it is mostly not noticeable in the results.

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Effects of vitiation and thermal boundary conditions on flame acceleration in microchannels: A numerical study

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Premixed hydrogen/air flame acceleration (FA) and the subsequent deflagration-to-detonation transition (DDT) of pure and vitiated fuel/oxidizer mixtures in a microchannel at two extreme wall thermal conditions – an adiabatic wall and a hot, preheated isothermal wall were numerically investigated. We employed AMReX-Combustion PeleC, an exascale compressible reacting flow solver that leverages load-balanced block-structured adaptive mesh refinement (AMR) to enable high-fidelity direct numerical simulation (DNS). We found that the FA rate and hence the DDT run-up distance to be strongly limited by the flame speeds of the unreacted mixture. Addition of water (i.e., vitiation) to the unreacted mixture leads to a significant reduction in the flame speed, thereby slowing down the FA process and subsequent DDT. With isothermal preheated walls, the pure fuel cases preferentially propagate along the wall after an auto-ignition event, leading to the formation of a "secondary" finger-flame which subsequently undergoes transverse expansion. The vitiated fuel cases also exhibit a similar behavior, nonetheless exhibit much longer time-scales of auto-ignition and propagation.

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A computational singular perturbation-based assessment of chemical models for two-dimensional hydrogen detonation simulations

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Detonation simulations are challenging due to the wide spectrum of characteristic length and time scales to resolve. In numerical simulations, the required time step is dictated by the stiffness of the chemical model. In this study, we examine 11 different hydrogen chemical models using Computational Singular Perturbation (CSP) technique to identify their smallest time scales (τ_min), with constant volume reactor. The conditions employed in the CSP analyses are determined from the post-shock (von Neumann states) of Zel'dovich von Neumann Döring (ZND) simulations relevant to H2-O2-3.76Ar. Grid convergence analyses of unsteady one-dimensional (1D) simulations, conducted with our in-house OpenFOAM solver in shock-attached frame of reference, reveal that the required grid resolution is inversely correlated with the smallest time scales identified in the CSP analysis. Simulations conducted with Mével 2017's and Burke 2012's chemical models, for which $\tau\_min \sim 1$ ns, are grid-independent when 48 points per induction zone length (pts/Δi) are employed, while at least 200 pts/Δi are required with Mével 2023's chemical model (for which $\tau\_min \sim 0.05$ ns). Due to the close agreement of Mével 2023's model with recent experimental measurements of Δi, grid convergence analysis is conducted with Mével 2023's model in two-dimensional (2D) simulations. In agreement with the 1D results, significantly finer grid resolutions, as compared to the typical 20 pts/Δi, are required to obtain a grid-independent solution with such stiff detailed chemical model. Such findings are relevant for the numerical simulations of detonations with any chemical system for which stiff chemical models are employed.

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Track11 Gas turbines, engines and furnaces

Track11-1 Gas turbines, engines and furnaces (1)

Chair: Masayasu Shimura
Wednesday, May 8; 13:30 - 15:10; Room M

Numerical investigation of effects of ammonia energy fraction and equivalence ratio on emission characteristics of ammonia/diesel dual fuel engine

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Emission characteristics of ammonia/diesel dual fuel engine is studied by LES with detailed chemical kinetic solver. Otomo mechanism for ammonia and ERCv2 for n-heptane are used in this study. LES is operated under several conditions with different ammonia energy fraction up to 94% and equivalence ratio conditions up to 0.91.

The simulation results show that unburnt ammonia and N2O are reduced simultaneously with increasing ammonia fraction, while NO is increased. Vice versa with decreasing equivalence ratio.

As for the higher ammonia energy fraction condition, conditional mean statistic show that a rise of adiabatic flame temperature due to the increase of ammonia equivalence ratio enhances (i) consumption of ammonia which is released from narrow space such as crevice of piston top ring while expansion stroke, (ii) decomposition of N2O in burnt region by reaction N2O(+M)=N2+O(+M) which has higher temperature dependence among N2O related major reactions, and (iii) production of NO in burnt region while NO in reaction zone is almost the same as the lower ammonia energy fraction condition.

The comparison between simulation results and actual engine test results showed that the simulation reconstructs the tendency of aforementioned exhaust gas change, which suggest the validity of the simulation.

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Exploring the Physical Significance of Robust Wiebe Function Parameters Through the Application of Artificial Neural Networks to Enhance the Analysis of Combustion in Internal Combustion Engines

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In the present study, the artificial neural network (ANN) has been utilized to combine the CFD (3D) and 0D models by training the neurons through the results obtained from the validated CFD model to estimate the parameters of a modified Wiebe function. The new and robust triple Wiebe function used in the present study is modified to exclude the assumption of arbitrarily selecting the value of efficiency parameters. The value of the correlation coefficient (R) for the training, testing, and validation is obtained as >0.99 for the estimation of Wiebe function parameters for each of the three combustion stages, which justifies the predictability of the present model. The physical interpretations of Wiebe function parameters corresponding to engine operation parameters (load, speed, compression ratio, fuel injection timing, and fuel spray angle) have also been studied. The results suggest that the present robust Wiebe function parameters can be satisfactorily used to map the engine operating parameters as well as performance parameters; therefore, the trained ANN model can be effectively used to optimize the engine performance parameters.

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Low Carbon Industry: Electrification of industrial processes involving high temperatures

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Industries are responsible of 26\% of the global CO2 emissions in the world in 2022 [1]. Therefore, this sector must reduce that figure to reach our sustainability goals by 2050. One possible path of decarbonization could be electrification of some fossil fuel intensive processes.

However, electrification cannot match the temperature requirement in all processes. Here the slab reheating furnaces used in the steel industry are considered.

The parameters that define the quality of the final product exiting these furnaces, used for thermal treatment, are the atmosphere composition and slab temperature. Therefore, reheating furnaces have a final low power zone, the soaking zone, to control the parameters mentioned before. This work studies the influences of the electrification of the soaking zone on the atmosphere composition and slab temperature. It investigates the use of electric heating elements instead of natural gas burners in the soaking zone. This has been done by comparing experimentally validated CFD results of a conventional slab reheating furnace model with CFD results of the hybrid furnace model where electrification goes up to 5MW in the soaking zone. Results show that the crucial process linked parameters remain similar (maximum 2\% variation) to the conventional process.

[1] IEA (2023), CO2 Emissions in 2022, IEA, Paris https://www.iea.org/reports/co2-emissions-in-2022, License: CC BY 4.0

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Identification of recirculation zones from experimental images of trapped vortex combustors using deep learning

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Trapped vortex combustors (TVCs), with potential applications in stationary gas turbine engines and compact aero-engines, exhibit a steady and locked primary recirculation zone (PRZ) in the cavity. It functions as a continuous source of enthalpy and radicals for combustion, contributing to enhanced combustion efficiency. Identifying the PRZ is critical for studying the combustion dynamics of such devices, an exercise typically conducted using particle image velocimetry (PIV) data. However, using tracer particles seeded into the fluid flow for measurements might introduce inaccuracies, especially in reacting flows. The consequences include the smearing of high-temperature gradients and the seed particles clogging the nozzles, thereby altering the effective inlet velocity of the fluid. To mitigate this, we investigate coupling a non-invasive diagnostic technique like OH chemiluminescence with deep learning to estimate the velocity components of large scales concerning the PRZ. After training and validating the model on datasets from large eddy simulations, we test it on snapshots obtained from simultaneous PIV and PLIF measurements. A satisfactory agreement between network outputs and ground truth has been observed in terms of the mean squared error and PDFs. Such models lay the foundation for intelligent data assimilation from experiments and simulations.

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Track11-2 Gas turbines, engines and furnaces (2)

Chair: Matthias Ihme
Wednesday, May 8; 15:30 - 17:10; Room M

Impact of excess air factors as a combustion parameter on NOx emissions in a 207 MW model industrial furnace

Mansur Aliyu
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The environmental impact of NOx emissions is substantial, leading to various adverse effects. NOx, comprising primarily nitrogen dioxide (NO2) and nitric oxide (NO), emerges as pollutants from combustion processes in power plants, vehicles, and industrial facilities. Recognizing the detrimental influence of NOx on the environment, the implementation of specific emission control technologies becomes imperative to mitigate its harmful effects. This study investigated the impact of operational parameters, specifically the excess air factor (α), on the NOx emissions from a 207 MW model industrial furnace used for steam generation in a boiler. The numerical approach employed for this investigation utilized ANSYS-Fluent. The study focused on a blended fuel composed of a mixture of methane and hydrogen. The governing equations, developed based on physical principles and assumptions, were solved using various models, including turbulent k-ε, species transport with the eddy dissipation concept for chemistry, and a NOx formation model. The findings of the study revealed robust correlations between α, temperature, and NO emissions. An increase in α led to a decrease in both the average furnace temperature and average NO emissions at the exit. Specifically, a 27% increase in α resulted in approximately a 55% reduction in NO emissions.

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Elucidation of heat transfer characteristics and NOx reduction phenomenon of elliptical radiant tube

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The radiant tube is an indirect heating device which transfers the heat of combustion inside the tube to the steel plate by radiation from the outer surface of the tube. The radiant tube is easy to maintain in the non-oxidizing or the reducing atmosphere around the object to be heated, so many industrial furnaces adapt to the radiant tube. On the other hand, since the heat of combustion is generated in the closed space in the tube, the tube often is creep-deformed at high thermal load. As a countermeasure against this deformation, the rigidity in the deformation direction is enhanced by making the shape of the radiant tube elliptical. In addition, the elliptical radiant tube having the same short diameter as diameter of the circular radiant tube increases the surface area and improves the heat transfer efficiency compared with the circular radiant tube. In this study, combustion characteristics and heat transfer characteristics of elliptical radiant tube were investigated using three-dimensional numerical simulation. As a result, the elliptical radiant tube obtains the same or higher thermal efficiency compared with the circular radiant tube. In addition, in the elliptical radiant tube, NOx emission is lowered in comparison with the conventional circular radiant tube.

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Development of a DEM-CFD coupling simulation for the stoker type waste incinerator

Ryusei Hayatomo, Tomohiro Denda, Takashi Nakayama, Takahiro Matsumoto
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In our company, we have analyzed the combustion of a stoker type waste incinerators using Computational Fluid Dynamics (CFD) simulations and utilized the results to improve furnace design and operation.

Recently, the performance requirements for incinerators, such as increased combustion stability and power generation efficiency, have become more advanced, therefore more detailed and accurate simulation of furnace phenomena is needed. In response to this, we are developing on the combustion simulation technology that coupling CFD and Discrete Element Method (DEM).

DEM is a method used for discrete calculations of particle behavior, and has been attracting attention to analysis techniques coupling with CFD because the computational cost has been greatly reduced by recent improvements in computer performances. When applying DEM to simulate the combustion in stoker type waste incinerators, we simulate the transport behavior of waste within the furnace by representing the waste as particles, and we also calculate the evaporation, volatilization, and solid combustion of the waste. By coupling these calculation results with the gas combustion results obtained from CFD, our final goal is to obtain a more detailed and accurate simulation results of overall furnace combustion phenomena. In this presentation, we will report on the status of our development.

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Numerical Investigation of CH4/O2/CO2 premixed flames stabilized over a dual annular counter-rotating swirl burner

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Abstract: This study investigates oxy-methane (CH4/CO2/O2) premixed flames within a dual annular counter-rotating swirl (DACRS) burner using numerical simulations. The burner structure comprises two concentric tubes: an inner tube for primary gas flow and an outer annular area for secondary gas flow. Maintaining a constant oxygen fraction (OF) of 34 vol % in both primary and secondary streams, the primary gas stream velocity is set at 5 m/s, while three secondary velocities (1.289, 1.667, and 2.2 m/s) are explored to analyze flow-flame interactions at different velocity ratios (3.878, 3, and 2.27). The Ansys-Fluent 2022-R1 software utilizes the partially premixed combustion model to simulate the reaction kinetics of the produced stratified flames within a three-dimensional periodic domain. Thermochemical properties and reaction rates are averaged using a probability density function (PDF) model. Validation against experimental data includes axial and radial temperature profiles and OH* concentration maps corresponding to visual flame appearances. The findings underscore highly effective interactions between the flame and airflow, yielding thorough combustion and notably diminished emissions within the DACRS stratified flames.

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Track11-3 Gas turbines, engines and furnaces (3)

Chair: Reo Kai
Thursday, May 9; 09:50 - 12:30; Room I

Evaluation of Preferential Diffusion in RANS Simulation of H2-Air Turbulent Flames with FGM Model

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The use of hydrogen as a fuel has gained significant attention for reducing CO2 emissions in high-temperature industries such as steel and aluminum production. However, hydrogen exhibits special combustion characteristics that differ from conventional hydrocarbon fuels, such as high reactivity and diffusivity. Therefore, the utilization of pure hydrogen as fuel requires significant modifications to existing combustion systems. In this context, Computational Fluid Dynamics (CFD) simulation is an essential tool for understanding, designing, and optimizing technologies operating with hydrogen. Reynolds-Averaged Navier-Stokes (RANS) RANS simulations are generally preferred for engineering applications involving complex and large-scale geometries due to the lower computational cost. Accurately modeling hydrogen combustion is challenging, particularly within the RANS simulations framework, since combustion models are mainly developed assuming unity Lewis number, ignoring effects such as preferential diffusion.

This paper presents a preliminary assessment of the effect of non-unity Lewis numbers in RANS simulations of H2-air turbulent flames by utilizing a recently developed version of the Flamelet Generated Manifolds (FGM) model that includes preferential diffusion. This FGM model accounts for mixture-averaged transport in the flamelets computed to construct the manifold and introduces additional diffusion terms to the transport equations of the controlling variables. Numerical simulations of hydrogen turbulent flames are conducted with and without considering preferential diffusion to observe its effect on the mean flame fields. Furthermore, a comparison with detailed chemical Direct Numerical Simulation (DNS) enables us to examine whether using a β-shape Probability Density Function (PDF) to model the turbulence-chemistry interaction is adequate for lean premixed hydrogen flames, where synergistic interactions of thermodiffusive instabilities and turbulence are present.

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Hydrogen combustion and NOx generation characteristics for a scaled hydrogen-fueled gas turbine combustor for aircraft propulsion

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Hydrogen combustion is one of the promising combustion methods for gas turbines to achieve carbon neutrality. Hydrogen has several particular combustion characteristics such as high flame speed and high flame temperature, and thus its behavior should be well understood for applications in aircraft engines. In this study, combustion and NOx generation dynamics of hydrogen flame is investigated in the LES framework. The thickened flame model is used to characterize the chemistry. The target combustor is JAXA's mode combustor which has multiple small-scale swirl-stabilized injectors, which quickly mixes hydrogen and air in the upstream region. The ambient pressure and equivalence ratio are varied to see the effect on exit temperature and NOx generation. Due to recirculation, a stable flame is formed and NOx generation occurs after some resident time. The pressure effect on the exit temperature is not strong and NOx generation is mostly correlated to local temperature. The effect of reducing the flow temperature by modulating the equivalence ratio on NOx generation is also discussed.

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Combustion and emission characteristics of oxy-syngas O2-CH4/H2/CO flames in a swirl premixed model gas turbine combustor

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This study investigates numerically the combustion and emission characteristics of CH4/H2/CO syngas flames in a swirl premixed model gas turbine combustor under oxy-combustion conditions for ease of exhaust CO2 capture. Simulations were performed over wide range of syngas composition at fixed inlet velocity of 6 m/s, equivalence ratio of 0.42, and oxygen fraction (OF) of 60%. The model was validated against the experimental data recorded on the same physical combustor setup. The results showed that increasing the hydrogen fraction (HF) from 0 to 80% of the syngas while keeping the remaining percentage of the syngas mixture equally divided between CO and CH4, a decrease in thermal power (TP) from 4.0 to 3.7 Kw, a rise in adiabatic flame temperature (AFT) from 2312 to 2388 K, a rise in laminar flame speed (LFS) from 0.53 to 1.32 m/s, and a decrease in power density (PD)

from 2854 to 2672 kw/m3 are observed. Excluding CH4, a decrease in AFT from 2447 to 2560 K, a decrease in LFS from 2.01 to 0.46 m/s, an increase in TP from 3.64 to 4.1 Kw, and increase in PD from 2620 to 2923 kw/m3 were obtained when decreasing HF from 90% to 10%.

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Turbulent combustion model sensitivity in LES of model gas-turbine combustor

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In this study, a model gas turbine combustor featuring a premixed swirl-stabilized flame is simulated with finite rate chemistry Large Eddy Simulation (LES). The design, originating from the Swedish National Center for Combustion Science and Technology (CECOST), aims to replicate the flow and flame features of an industrial gas turbine combustor under atmospheric conditions. A 10.5 million cells hexahedral grid with local refinement in critical regions is used. The simulations, performed in OpenFOAM, target a lean, stable, methane-air flame. Using the pathway centric 42 step reaction mechanism of Zettervall et al. together with the Eddy Dissipation Concept (EDC), Partially Stirred Reactor (PaSR), and Quasi Laminar (QL), combustion models we assess the influence against experimental data, through OH- and CH2O-PLIF, as well as PIV measurements. Good qualitative and quantitative agreement is obtained but differences between models are also observed in temperature and species distributions, impacting flame characteristics and dynamics. Notably, the EDC displays a more intense, more compact flame with effective stabilization, while PaSR exhibits complex dynamic phenomena involving large-scale fluctuations of the flame front. Findings emphasize the sensitivity of lean methane-air flame simulations to combustion model selection, with implications for broader applications where model differences may rival those from distinct alternative fuels, or operating conditions.

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LES of spray combustion in a lean direct injection combustor using a novel subgrid-scale stress model

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Large eddy simulation (LES) of spray combustion is an important tool for developing and designing new-generation aero-engine combustors, and various subgrid-scale (SGS) closure models for LES have been developed. Turbulent combustion, accompanied by strong turbulence-combustion interactions, plays an important role in aero-engine combustors. However, the influence of combustion on turbulence is rarely considered in previous SGS turbulence modeling. In the present work, we develop a novel SGS closure model considering combustion effects and name it the flame surface and k-equation based gradient model (FKGM). LES of spray combustion in the NASA Lean Direct Injection (LDI) combustor is conducted to validate the FKGM model and analyze the complex spray flame structure. The FKGM model achieves better agreement with the experimental measurements compared with the dynamic Smagorinsky model (DSM) in terms of gas mean and fluctuating velocities, which indicates the model's accuracy. Radial profiles of temperature, major combustion products, and droplet diameters are also well reproduced in the current simulation. The inner recirculation zone (IRZ), small outer recirculation zones, and three main flame zones are well captured. The flame index is introduced to identify different combustion regimes in the complex spray flame where both premixed and diffusion regimes coexist. Quantitative statistics related to the heat release rate show that the heat release intensity of the premixed flame regime is higher than that of the diffusion regime.

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Large eddy simulations for investigating combustor-turbine interaction: a machine learning approach to reduce discrepancies between single-component and multi-component simulations

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The aerodynamic and combustion interaction across the combustor and axial turbine in a micro gas-turbine engine is studied by a high-fidelity 360 degree azimuthal large-eddy simulation. By comparing with the standalone combustor or turbine cases, the fully coupled combustor-turbine simulation shows a significantly different flow field. Coupling with the axial turbine downstream, temperature uniformity (OTDF) near the combustor exit increases, which causes severe hot streaks on the turbine blades. Next, we apply the distribution of total temperature and pressure obtained from the interface of coupled combustor-turbine simulation to the outflow/inflow boundaries of the standalone combustor/turbine cases. The results thereby show the aerodynamic and combustion predictions of standalone cases now switch to be consistent

with the coupled combustor-turbine results.

As multi-component simulations are not very effective in the engineering field, people are used to conduct single-component simulations for research and design. In this work, we propose a machine learning method to approximate single-component results to the multi-component simulation. A convolutional neural networks (CNN) approach to train the trivial outflow/inflow boundary conditions of standalone combustor/turbine cases, to obtain the interface distributions of the multi-component simulations in a range of operation conditions (different mass flow rates and pressures) and varying installation angle of the turbine stator blades. The CNN predicted interface can thus be applied as new outflow/inflow boundary conditions for the standalone combustor/turbine cases to approximate the multi-component simulation results with an excellent generalisation.

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Effects of Detailed Chemistry and Molecular Differential Diffusion on a Reacting Jet in Cross-Flow

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Significance of a jet in cross-flow (JICF) lies in practical applications in combustion systems, like gas turbines, emission controls of pollutants resulting from incomplete mixing, and aircraft engine performance for higher thrust capabilities. In this study, we simulate three distinct JICF scenarios: non-reacting (NR) and two reacting cases (R1 and R2). In the R1 case, the flame exists external to the jet shear layer, while in the R2 case, the flame resides within the jet shear layer. To achieve this, we employ our in-house reacting flow solver developed based on OpenFOAM and Cantera, to investigate the impacts of detailed chemistry, mixture-averaged transport models, and vorticity structures within cases. Specifically, we demonstrate the following: (i) A single-step chemistry model demonstrates reduced jet velocity, resulting in notably weaker shear layer vorticity formations and the presence of narrow, high-endothermic lines. Conversely, the detailed chemistry setting portrays wider endothermic areas without a flame on the windward side. (ii) Detailed mixture-averaged transport models can exhibit an attached flame for R1 and R2 cases, consistent with experimental results. (iii) The vorticity structure analysis shows shear layer vorticity, horseshoe vorticity, and counter-rotating vortex pairs depending on a ratio of the crossflow and jet flow velocities.

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Track11-4 Gas turbines, engines and furnaces (4)

Chair: TBD
Friday, May 10; 09:50 - 11:50; Room I

Prediction of heat release and wall heat transfer in a scramjet combustor via Pareto-efficient combustion modeling

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Modeling supersonic combustion presents significant challenges for tabulated chemistry approaches, leading to inaccurate reconstruction of the thermochemical state, chemical species, and heat release rate. Furthermore, tabulated chemistry models perform poorly near walls, where nonadiabatic conditions and recombination reactions cause inaccurate heat flux predictions. We extend the Pareto-efficient combustion (PEC) model to supersonic combustion and simulate the RC19 scramjet combustor. Sensitivity analysis is performed to determine chemical species most strongly impacting the heat release prediction. By appropriate selection of the parameters of the PEC model, we show that accurate predictions of total heat release and wall heat transfer may be recovered via application of finite-rate chemistry to less than 15% of the computational domain.

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Numerical modelling of combustion stability prediction in a dual mode ramjet with a cavity flameholder

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The renewed interest of the aeronautics industry in hypersonic propulsion systems led to new experimental studies of dual mode ramjets (DMR). Still, the transition from supersonic to hypersonic regime could show an oscillating behavior as the combustion shifts from subsonic to supersonic. However, experimental data is still scare in the literature. Computational Fluid Dynamics (CFD) represents a viable alternative to study the behavior of such engines. Where cold flow simulations could be considered as predictive, the combustion process and stabilization is more complex to capture. In this context, the Partially Stirred Reactor (PaSR) model is evaluated in the DMR context.

To this end, 2D and 3D RANS simulations are performed on a cavity-based scramjet. The PaSR model is compared to both the tabulated chemistry assumption (FGM) and the Eddy Dissipation Concept (EDC) model, another reactor-based model. The results of the simulations show an improved prediction of both the backpressure and the flame anchoring locations. Furthermore, 3D effects are investigated together with a sensitivity analysis of the chemical timescale formulation.

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NOx Formation Analysis Applying Clustering Method using Adversarial Autoencoder to numerical results on Hydrogen-Rich Ram Combustion with LES

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NOx formation in a hydrogen-fueled model ram-combustor for a Pre-Cooled TurboJet (PCTJ) engine which operates afterburner in hydrogen-rich conditions was numerically investigated with Large Eddy Simulation (LES). For comparison, analysis in hydrogen-lean conditions was also conducted. Combustion proceeded faster in rich conditions than in lean conditions due to the larger momentum ratio of fuel jet to mainstream air. The LES results which are multi-dimensional and large-size data were mapped to the 2D latent space and classified into 7 classes by Adversarial AutoEncoder (AAE) which is one of the deep clustering methods using a generative model. The contributions of the main NOx formation routes in each class were calculated. It was shown that almost all NO was formed by the thermal NO route in reaction zones and high-temperature air-side diffusion layers. It was also demonstrated that NO was reduced in hydrogen-rich burnt gas and fuel side diffusion layers because there are H and NH radicals and few O radicals. It was concluded that hydrogen-rich combustion was advantageous for hydrogen-ram combustors in terms of quick completion of combustion and NO reduction in burnt gas. Additionally, it was also confirmed that AAE clustering was effective in NOx formation investigations in complex combustion fields.

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Wavelet optical flow velocimetry of a scramjet combustor using high-speed frame-straddling focusing schlieren images

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Velocity field measurement under extreme conditions such as a scramjet engine presents great challenges, featuring ultra-high-speed turbulent reacting flow, high-temperature with intense luminescence. The present work demonstrated a seedless velocimetry approach using focusing schlieren images (FSI) of high spatiotemporal resolution in a scramjet engine. Two fuel mass flow rates were investigated with corresponding global equivalence ratios of 0.27 and 0.13, respectively. The FSIs enabled by the employment of a high-speed pulsed LED light source are characterized by an effective exposure of 100 ns, and a 500-ns frame-straddling time interval with a full resolution recorded at 76 kHz. The 100-ns exposure allows for capturing of transient high-speed flow motion without blurring, and the 500-ns time interval ensures an appropriate spatiotemporal correlation between subsequent schlieren images for high-speed reacting flows. Wavelet-based optical flow velocimetry (wOFV) algorithm was developed and applied to the FSIs. In contrast to the correlation-based algorithms widely employed in PIV for distinct particles, wOFV algorithm turns to optimize a penalty function which suits better FSIs with continuous variation in brightness. The maximal velocities in the main duct of the scramjet combustor were measured to be approximately 550 m/s and 1100 m/s for two cases studied, suggestively corresponding to subsonic and supersonic combustion modes, respectively. Velocity inside the cavity is generally below 200 m/s for both cases. Recirculation regions and their dynamic motion inside the cavity were well resolved from the measured flow field at 38 kHz. In summary, the development of present velocimetry approach holds great potentials for applications in extreme flow conditions.

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A Bayesian optimization framework for the control of combustion instability of a bluff-body stabilized combustor

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Combustion instability is one of the significant problems affecting safety in modern gas-turbine combustors. Temperature and pressure peaks due to combustion instability are particularly harmful for the structural damage

they can cause as well as for performance degradation and increase of pollutant emissions. Control of combustion instability for a realistic gas-turbine combustor is challenging. This work aims to establish an efficient numerical framework for optimization to improve the combustion stability of a bluff-body combustor. High-fidelity large eddy simulations of the spray combustion process in the combustor are conducted and the experimental measurements are used to evaluate the numerical accuracy of the baseline case. The air preheating temperature, the Sauter mean diameter of fuel droplets and the location of liquid fuel injection are regarded as input variables. The rms of pressure is regarded as an optimization objective. The Bayesian optimization framework is proposed that includes the sampling process, surrogate model, acquisition function and genetic algorithm optimizer processes. It is found that Prms can be reduced by 86% for the optimized case compared to the baseline case using only 16 sample evaluations. The present framework is easy to be extended to multi-objective framework that considers the NOx emission as an additional objective. This work is promising as it provides an effective optimization framework for the development of next-generation gas-turbine combustors.

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Investigation of the simple CFD methods to predict the flame holder flow field of the hypersonic jet engines

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The development of hypersonic engines such as scramjet engines with high enthalpy flow requires large-scale test facilities, many hardware fabrication and testing trials, manpower, and time for these processes. Therefore, the application of CFD simulation is important to save the huge development cost and time. However, CFD analysis of such flow is not only technically challenging and needs huge amount of computer resources, but also the current prediction accuracy is not always enough. This makes the application to multi-objective optimization needed for speedy hardware design and development rather difficult. Therefore, the purpose of this research is to develop simple simulation methods that can perform supersonic combustion flow field calculations on a workstation. Since flame holding inside a hypersonic engine is a difficult and important technique, this research focuses on flame holders of the hypersonic engines. In order to accommodate various flame holder flow fields, two types of hypersonic engines were selected for simulation trial: A Rocket-Based Combined Cycle (RBCC) engine and a scramjet engine. For the results of the hypersonic wind tunnel tests and full 3D LES analyses, a computationally less demanding analysis methods combining an extremely thin 3D geometry model and a simple one-step chemical reaction model was applied. As a result, the combination of the appropriate modeling methods was able to qualitatively reproduce the pressure distribution in the RBCC engine and the mixing flow behavior inside the flame holder of the scramjet engine.

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Track12 Fires

Track12-1 Fires (1)

Chair: Sayaka Suzuki
Thursday, May 9; 09:50 - 12:30; Room E

Large-Eddy Simulation of aeronautical fire certification: coupling strategies for multi-physics modeling

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Fire certification stands as a crucial milestone in the aeronautical product development cycle. During this process, the component to be tested is exposed to a kerosene burner-induced flame for 5 to 15 minutes. The notable failure rates in fire resistance tests lead to long and costly development phases. Leveraging numerical simulation holds promise for comprehending the thermal impact of the flame and optimizing material design. These tools are essential in addressing emerging challenges, including evolving certification standards, the use of complex materials such as composites and assemblies, and the arrival of alternative fuels.

To this purpose, we present a methodology for Large-Eddy Simulation (LES) of certification burners, encompassing a wide range of multi-physics and multi-scale phenomena: turbulence, fuel injection and atomization, spray combustion, conduction within solid components, and conjugate heat transfers at the interface. This methodology couples a low-Mach number combustion solver, a solid solver, and a radiative solver, relying on the CWIPI library. With appropriate communications, solvers can independently but simultaneously address reactive processes within the flame, thermal conduction in a solid material, and radiative heat fluxes throughout the domain. Recent developments in numerical, meshing, and coupling strategies have significantly reduced the computational time of such simulations, thus enabling the application of the methodology to well-controlled fire resistance tests under various operating conditions and for different burners. Prediction of heat transfers is validated on a simplified test case by comparing the temperatures of a well-instrumented metal plate impacted by the flame.

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Large eddy simulation of turbulent tandem diffusion flames under crosswind conditions

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The interaction between fire sources and the response to cross airflow is one of the essential topics in the study of multiple fire sources. Large eddy simulations (LES) were performed for turbulent tandem diffusion flames under crossflow to study flame-flame interaction. The computational code was an in-house version of FireFOAM, a fire simulation solver within OpenFOAM. Turbulent combustion is modelled using the extended eddy dissipation concept for LES published by the authors' group. The dynamic Smagorinsky model is used for sub-grid scale modelling in LES. The experimental data were taken by one of the authors. The data were about propane fires from tandem burners, varying separation distances between fires (3D-5D, where D is a burner size of 15 cm) and heat release rates (17.43-34.86 kW). First, the computational results were validated using the measured flame width, and further investigation was carried out on the flame behaviour of the turbulent tandem diffusion flames under crossflow. Specific flame oscillating behaviour in the spanwise direction was observed, especially for a downstream diffusion flame, which was identical to the experiment. The flow field heavily influenced the behaviour of the flame and the wake structures behind it.

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Large-eddy simulation of a methane fire plume using steady and unsteady flamelet models

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An accurate prediction of fire dynamics is important for the assessment of fire safety and the design of fire protection systems. It is challenging to model fire plumes due to the complex interactions of multi-physics, including the buoyancy-driven turbulence, chemistry, fluid dynamics, radiation, and the transient effects of ignition and extinction. In this work, we will conduct large-eddy simulation to predict a one-meter diameter methane fire plume using steady and unsteady flamelet models, in which the radiation and transient effects are considered. The radiation effects are considered by solving the transport equation for the total enthalpy with the radiation source term in the flow solver, while the temperature boundary condition for the flamelet equations is varied to consider the radiative heat transfer. In the unsteady flamelet model, the flamelet solutions obtained from the unsteady flamelet equations are parameterized as a function of mixture fraction, progress variable, scalar dissipation rate, and total enthalpy. The turbulence-chemistry interactions are considered with proper presumed probability density functions. The performance of the flamelet models in predicting the pool fire will be evaluated by comparing against the available experimental data. In particular, the transient effects will be analyzed in detail.

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Feasibility of a simple dust-explosion model to predict limit conditions

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Explosions can occur wherever combustible dust is handled, and information on limit conditions, such as the minimum explosive concentration (MEC) and the minimum ignition energy (MIE), is crucial for developing safety measures. Although extensive experiments have been conducted to report these data, controlling experimental parameters, such as particle diameter and dust concentration, is challenging, making numerical predictions attractive alternatives. This study examines the feasibility of a simple dust-explosion model to predict limit conditions. The model ignores the gas-phase density variation due to combustion, as in the constant-density approximation frequently used in analyzing gaseous premixed flame propagation. This approximation, along with the assumption of point heat sources, enables the use of fundamental solutions, significantly reducing the computational cost. Predicted burning velocities and the minimum explosive concentration are compared with available experimental data to test the model's validity for predicting practically useful information.

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Flame retardant effects on non-premixed boundary layer flames

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In fire scenarios, boundary layer flames (BLFs) can develop at flammable, "active" walls and they are fueled by volatiles released during the thermal degradation of the wall material. In this context, flame retardants (FRs), integrated into materials like polymers, can play a vital role in fire mitigation. However, their influence on BLFs dynamics remains inadequately explored. In this work, we aim to address this gap by numerically investigating BLFs under the influence of FRs. We first conduct a combined experimental and numerical investigation of non-premixed methane-air flames at an active wall. A novel flame configuration is employed, featuring a primary premixed flame in a side wall quenching configuration, with methane injected through a secondary wall inlet above the flame's quenching point. The secondary diffusion flame transfers heat to the wall resulting in a complex thermochemical state. The latter is analyzed for different mass flows issued from the wall inlet and implications for reduced order modeling/manifold generation are identified. Furthermore, we examine the influence of phosphorus-based FRs on the structure of the non-premixed BLF and the induced changes to the thermochemical state. The present work provides insights into FR-BLF interactions, contributing to the development of more effective fire safety measures.

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Simulation study of fire dynamics and heat transfer: the effects of wind and slope

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The slope and wind speed are deemed to be the determinant factor driving the eruptive spread of wildfire, which

however has not been fully investigated. A systematic study is therefore carried out to quantitatively characterize the fire behaviors with varying wind and slope conditions, for which the physics-based numerical simulations are performed. The rate of spread increases with increasing both slope and wind speed, but an abrupt growth is exhibited when slopes are larger than 20°. At higher slope, the fire line also experiences the transition from a U-shape to a pointed V-shape, along with the appearance of the stripe burning zones, indicating a faster spread but incomplete combustion. Conversely, for low wind speed and slope conditions (≤ 10°, ≤ 1.0m/s), an interesting deformation of fire front into a W-shape is observed, which is attributed to the combined action of lateral air entrainment and the backflow in front. It is also revealed that at high slope conditions, the convergence of incoming wind stream and the weakened indraft flow contribute significantly to the eruptive fire spread. Different mechanisms are identified for the heat transfer ahead of fire front, i.e., the radiative heat is mainly affected by the enlarged volume of fire plume, and in contrast, the flame attachment at high slope (especially for >20°) would dominates the convective heating for the acceleration of fire spread.

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Swift Flame-to-Fuel Heat Transfer Evaluation in Simulation via Deep Learning and Fire Images

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In the realm of numerical fire simulations, the intricate calculation of thermal feedback from the flame to the solid or liquid fuel surface stands as a pivotal factor, bridging the gap between gas-phase flame combustion and condensed-phase fuel gasification. However, within CFD fire modeling tools, this computation proves computationally demanding due to the necessity for a high-resolution grid to compute interface heat transfer. This study introduces a groundbreaking approach—a real-time prediction of flame-to-fuel heat transfer using computer-vision deep learning and simulated flame images. The model is trained using images from various methanol pool fires, offering insights into the shift from convective to radiative heat transfer as pool diameters increase from 20 cm to 40 cm. Results showcase the AI algorithm's ability to predict both convective and radiative heat flux distributions on the condensed fuel surface in real-time, leveraging flame morphology captured by a larger grid. This innovative method, applicable to diverse fire scenarios, goes beyond empirical correlations to predict non-uniform heat transfer coefficient distributions on the interface. The study demonstrates the efficacy of AI and computer vision in accelerating complex numerical fire simulations, enabling the modeling of intricate fire behaviors with reduced computational expenses.

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Track12-2 Fires (2)

Chair: Samuel L. Manzello
Friday, May 10; 13:00 - 15:00; Room I

Numerical study of pyrolysis, flaming and smoldering of wildland fuels using detailed kinetics coupled with a multi-region single-particle model

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Wildland fires have been responsible for the destruction of vast amounts of infrastructure, thus yielding massive damage. They are also a major global source of greenhouse gas emissions and aerosols, which have significant impacts on air quality and climate. In this context, a fundamental understanding of the burning processes of wildland fuels is crucial for the modeling and prediction of both fire behavior as well as related emissions. This work leverages a novel multi-dimensional combustion kinetics solver to investigate the pyrolysis, flaming and smoldering combustion of biomass, considered as a common wildland fuel surrogate. Biomass fuels are represented through their fundamental constituents, such as lignin, cellulose, hemicellulose, water, and extractives. A detailed reaction kinetic model is adopted to reproduce the process of their degradation, including char oxidation. Validation of the modeling framework with experimental data from literature is performed at various scales, including thermogravimetric experiments and particle-scale experiments of pyrolysis and combustion. The goal is to evaluate the dependency of emissions on potentially influential parameters, such as flame temperature, atmosphere conditions and particle size. These results will then be used to construct sub-models for large-scale wildfire applications.

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A model for fire growth and suppression of thin melting plastics in FireFOAM

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Industrial fires may feature thermoplastics with thin constructions and complex geometries that readily melt and deform. This behavior is too complex to directly represent in large-scale computational fluid dynamics (CFD) fire simulations such as those performed in FireFOAM, and so we present a simplified model that captures the leading order physics and provides a computationally tractable implementation. In this approach, we approximate the initially solid plastic as thin, geometrically 2D surfaces. Each face on the surface evolves a pseudo-1D conservation of mass and energy equation coupled with the gas-phase CFD, Lagrangian parcels for molten plastic (due to dripping/impingement) and water (due to sprinkler spray). The pseudo-1D equations account for: convective and radiative heat transfer from the fire; melting/solidification and gasification of the initially solid plastic; and dripping and impingement of both molten plastic and water. The plastic surface is treated in a dynamic manner, allowing for remeshing where plastic elements have collapsed, reflecting the real-world geometry changes that impact various heat/mass transfer processes. The fire growth part of the model has been validated against full-scale experiments and the suppression part is demonstrated here for the first time.

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Numerical Simulation of Flame Spread on an Inclined Thin Paper using the Fire Dynamics Simulator (FDS)

Shinnosuke Nishiki
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Understanding the complex mechanisms of fire spread is crucial for preventing fire damages. Experiments indicate that when paper is inclined, the flame spreads downward over a specific range of slopes. This study shows that numerical simulation using FDS (Fire Dynamics Simulator) reproduce such of experimental results. Particularly when incline is 35 degree and gap is 3mm to the bottom boundary, after igniting in the center of an inclined paper, the flame spread downward in a fan shape. Reaching flames the bottom edge, the top half part is burned quickly. This situation very well reproduces what was observed in experiments. During the fan-shaped flame spread, the distribution of high temperature and total heat flux on the paper surface is concentrated near the tip on the descending side of the flame propagation. There is sufficient heat flowing into the paper to cause thermal decomposition, and the sufficient of oxygen supplied is also sufficient, so combustion continues. At that time, the upper side of an inclined paper, the inflow of heat is insufficient and the supply of oxygen is also insufficient, resulting in slow combustion. After burning out downward, the enough oxygen supply prompts the flame to spread upward. Calculations for different gradient/gap conditions between paper and ceramics have been run to confirm that the experiment can be reproduced and to elucidate the phenomenon.

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Numerical Investigation on the Effects of Char Oxidation in Near-limit Flame Spread over a Solid Fuel in Microgravity

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Experiments have reported that the flame over a solid fuel breaks into flamelets in a near-extinction microgravity environment and extends the range of material flammability. However, the role of char oxidation in flamelet behaviour is little known so far. Thus, an elaborate 3D numerical model of one-step, second-order global gas-phase reaction between fuel vapour and oxygen solving mass, species, momentum and energy conservation equations, with a simultaneous char model consisting of char formation and oxidation, first-order Arrhenius pyrolysis model in solid phase solving mass and energy conservation equations in a the flame-fixed coordinate system with thermal radiation calculated using the Discrete-ordinates method coupled with a grey model for the radiative properties of Carbon dioxide and Water used to investigate the effects of Char Oxidation in near-extinction conditions. The heat feedback from Char Oxidation is expected to assist in sustaining the flamelets and extending the range of material flammability.

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Track12-3 Fires (3)

Chair: Shinnosuke Nishiki
Friday, May 10; 15:20 - 17:20; Room I

Role of Numerical Combustion for Improved Understanding of Wildland-Urban Interface (WUI) Fires

Samuel L. Manzello[1], Sayaka Suzuki[2]
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The wildland-urban interface (WUI) fire problem is continuing to spread all over the world. Due to continued changes in global climate, many areas not often associated with a WUI fire problem are now being forced to deal with this new challenge. The fire research community have developed computational fluid dynamic (CFD) models that have mainly been validated for fires that occur inside buildings. The wildland fire community have developed operational models that are being used by fire management personnel to try to make global decisions on fire spread processes. A broad overview of research-based and operational models for WUI fires will be presented. The talk will then move into recent experiments by our group needed to model complex firebrand accumulation processes, missing from current models. The firebrand generator, which has the ability to make a firebrand shower, was used to recreate firebrand accumulation processes seen in real WUI fires. Detailed analysis was performed to understand the complex firebrand accumulation processes.

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CFD analysis of tunnel fire under rainfall using species-transport and discrete phase model

Dia Luan[1], Jakub Bielawski[2], Xinyan Huang[3], Chuangang Fan[1]
[1]Central South University, China, [2]Building Research Institute, Poland, [3] The Hong Kong Polytechnic University, China

The study of fire in a tunnel is crucial for fire safety. This work underscores the significance of Computational Fluid Dynamics (CFD) techniques in addressing the interaction between fires and rainfall. The dynamics of a tunnel fire under rainfall have been simulated using FLUENT software from ANASY Inc. Discrete phase model based on the Lagrangian approach and the species transport model considering chemical reactions are applied to the simulation of rain and fire, respectively. The computational domains, boundary conditions, solution strategy, and solve setting are outlined. This work focuses on the flow flow, temperature fields, and turbulence characteristics, and simulation results are compared to model-scale tests. Different turbulence models are discussed and the ability of the Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) turbulence method to predict the unsteady flow field in unstructured grids is evaluated. Additionally, thermocouple models play a crucial role in addressing the prevalent issue of overpredicted temperatures in fire simulations conducted by FLUENT. This work supports the effectiveness of CFD techniques in simulating fires and provides some recommendations for CFD modeling of tunnel fires.

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Accelerating Tunnel Fire Simulation: A Comprehensive Approach Integrating CFD and Deep Learning

Yuxin Zhang, Xinyan Huang
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This study pioneers an advanced approach to tunnel fire simulation by integrating computational fluid dynamics (CFD) and artificial intelligence (AI) using deep learning techniques. The simulation focuses on crucial fields for human behavior in fire, such as temperature, visibility, carbon monoxide (CO), and thermal radiation in tunnel fires.

The research firstly leverages the Fire Dynamics Simulator (FDS) for comprehensive scenario simulations across diverse tunnel and fire conditions. Therewith, the application of deep learning for time series prediction enables the extraction of dynamic fire development rules from the simulated scenarios. The resulting model facilitates real-time forecasts of the aforementioned fields based on specific tunnel and fire parameters. This AI-driven time series simulation approach offers a sophisticated tool for emergency responders and tunnel operators, delivering precise and adaptive insights to optimize evacuation strategies during tunnel fire incidents in real time.

The synergy of numerical simulations and AI applications using deep learning for time series forecasting represents a cutting-edge contribution to tunnel safety and emergency response. By harnessing the power of predictive analytics, this research not only advances our understanding of tunnel fire dynamics but also provides a practical tool for decision-makers to enhance overall tunnel safety and evacuation preparedness.

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AI-based fire smoke simulation for buildings with complex geometry

Yanfu Zeng, Tianhang Zhang, Zilong Wang, Xinyan Huang
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Fire-smoke modelling is a common practice for building design to assess the efficiency of proposed fire protection provisions, such as fire compartmentation and smoke extraction system. However, the current design process based on computational fluid dynamics (CFD) modelling is time-consuming and costly. This work aims to achieve a real-time prediction on the fire-induced smoke movement for buildings with complex geometries by applying artificial intelligence (AI) technology. A numerical building fire database containing different building geometries was first established, which was then trained by a generative adversarial network (GAN) model to learn the smoke movement patterns. By inputting the physical model of the building, the pre-training GAN model can output the soot visibility slices within seconds for 1MW T-square design fire. The result shows that AI can reproduce the descending process of the smoke layer from the perspective of vertical (X or Y directions) slices across the fire location, and also provide comparable smoke filling patterns from the view of horizontal (Z direction) slice at 2 m height above the fire. The prediction accuracies for five testing cases are between 83% to 96% except for one extremely innovative-designed building. This research verified the feasibility of using AI to predict smoke movement for complex buildings, which can significantly reduce the design cost and enable more cost-effective solutions.

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Linking Real Fires to Numerical Simulations with Image-Based Flame Identification

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In real fire scenarios, the Heat Release Rate (HRR) is often an unknown parameter, presenting a significant challenge in accurately simulating and replicating fire scenarios. This study introduces a novel approach for bridging the gap between real fire scenarios and numerical simulations through image-based flame identification. The primary focus lies in utilizing the identified Heat Release Rate (HRR) from flame images as a crucial input parameter for the Fire Dynamics Simulator (FDS). The proposed methodology involves the creation of a comprehensive image database derived from various fire tests conducted by National Institute of Standards and Technology (NIST), specifically chosen to encapsulate diverse fire dynamics. Subsequently, a computer vision-based deep learning model is employed to accurately identify and quantify the HRR associated with different flame morphologies. The identified HRR values serve as inputs for the FDS, enabling the numerical simulation to emulate real fire behavior with heightened accuracy. The efficacy of this approach is demonstrated across a spectrum of fire scenarios, ranging from growing and decaying fires to instances of puffing flames induced by buoyancy effects. The results showcase the capability of the developed image-based flame identification model to help simulate the real fire behaviors. This innovative methodology contributes to advancing numerical fire simulation by incorporating real-world flame characteristics, facilitating a more accurate and efficient representation of complex fire behaviors.

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Track14 New combustion technologies

Track14-1 New combustion technologies (1)

Chair: Amir Mardani
Wednesday, May 8; 15:30 - 17:10; Room H

Performance Characteristics of a Tangential Flow Burner for Ammonia Combustion

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Burning ammonia has recently gained considerable attention due to its high hydrogen content and zero carbon emissions. However, achieving a stable flame with pure ammonia is a challenging issue due to its low energy content and flammability limit. From an emissions standpoint, fuel NOx poses a significant issue with ammonia flames. In this study, we have developed a tangential swirl-based two-stage burner to maintain stable pure ammonia flames while minimizing NOx emissions. The unique burner design integrates both recuperative features and effective air staging. Experimental assessments were conducted across various equivalence ratios (0.5–1.2), spanning a thermal intensity range of 1.5–4.6 MW/m3. The factors considered in the burner's development are wall heat-loss effects, local mixing characteristics, and available ignition energy. Consequently, this novel burner achieved the lowest NOx concentration with zero ammonia emissions compared to those reported in the literature. To delve deeper into the burner, 3D numerical simulations using Large Eddy Simulations (LES) were performed to examine mixing characteristics, ammonia consumption, and NOx production rates. The findings revealed a well-distributed temperature profile, with the lowest NO production observed at higher thermal intensities. Notably, a specific NO level of 2.8 PPM/kW was identified at a thermal intensity of 3 MW/m3 and an equivalence ratio of 1.1.

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A numerical study of ammonia cracking in bluff-body stabilized non-premixed flames

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This study explores a novel in-situ ammonia decomposition approach in the recirculation zone of a newly designed bluff-body burner at KAUST. The application of this method improves flame stability and minimizes emissions. To gain improved fundamental insights, numerical simulations with Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulation (LES) reduced-order models, relying on parameterizations of the thermochemical state space, were employed, and their predictions are contrasted against recent measurements obtained at KAUST. Additionally, a potential enhancement of the modeling approach can be achieved by incorporating finite-rate chemistry (FRC) models. A key discovery of this study is the identification of two distinct zones within the burner: a lower luminous region characterized by intense burning and an upper flameless region exhibiting vitiated combustion, effectively consuming NO. Such findings highlight the potential of this approach as a promising avenue for mitigating environmental impact while enhancing ammonia flame stability.

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Low-order modeling of ammonia combustion in porous media burners

Thorsten Zirwes[1], Guillaume Vignat[2], Emeric Boigné[2], Matthias Ihme[2]
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Ammonia is becoming an important carbon-free fuel due to its production from renewably generated hydrogen and ease of storage. However, ammonia flames are characterized by low flame speeds and high ignition delay times, making it challenging to stabilize flames with high power density. One promising approach are porous media burners (PMBs). In this configuration, the flame burns within connected pores of ceramic foams. Heat

recirculation from the solid phase stabilizes the reaction zone and enables high power density combustion even of pure ammonia flames. While this has been successfully demonstrated experimentally, the numerical simulation of PMBs using low-order one-dimensional models still poses a challenge due to the complex multi-physics given by the interaction of the gas and solid phase. This includes heat conduction in the solid, radiation, heat transfer between the phases and modification of diffusive fluxes by the tortuosity. In this work, we present a 1D open-source solver (https://github.com/IhmeGroup/PMCToolbox) based on Cantera and extended for PMBs. The code is validated by considering the experimentally studied ammonia PMB. Using effective properties from µCT-scans of the solid structure, good agreement between simulation and measurement was found in terms of pollutant emissions and flame stabilization characteristics.

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New concept for aerodynamic stabilization of lifted hydrogen diffusion flames

Jakub Tumidajski, Adam Klimanek
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Hydrogen oxy-combustion offers a solution with water vapor as the sole combustion product, addressing emissions concerns. Challenges arise from the high temperature (3600 K) of hydrogen flame in pure oxygen, exceeding commonly used material thermal resistance. This high temperature gives rise to two problems: contact between the flame and the burner tip, and contact between the flue gas and the combustion chamber walls. Lifting the flame and introducing cold air mitigate these, but traditional burners risk flame instability, especially with varying burner power.

To overcome these challenges, a specialized burner is proposed. Configured for separate reagent delivery, angled oxygen injection forms a barrier, reducing fuel velocity for aerodynamic flame stabilization away from burner walls. Simultaneously, steam introduction between fuel and oxygen inlets ensures targeted intersection for optimal flame occurrence. The elevated temperature of steam facilitates spontaneous ignition and serves as a diluent for temperature control.

The study focuses on investigating hydrogen combustion in lifted diffusion flames under diluted conditions for gas turbine applications. Numerical simulations explore flame stability, considering parameters like dilution ratio, equivalence ratio, diluting gas inlet temperature, burner geometry, and dilution agent. Adjusting these parameters enables control over temperature, flame lift-off height, and achieving complete combustion, minimizing unburned fuel at the combustion chamber outlet. The objective is to provide insights into combustion physics, guiding the design and operation of the hydrogen burner for a mixed gas/steam turbine cycle, aiming at emission reduction and efficiency improvement.

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Combustion and emission characteristics of a premixed NH3/O2 jet flame in hot coflow of N2 versus H2O

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Ammonia is a promising alternative carbon-free fuel, but its conventional combustion is unstable and emits lots of NOx. Moderate or intense low-oxygen dilution (MILD) combustion features high stability and ultra-low NOx emissions, and the addition of H2O can further reduce NOx formation. The present work numerically investigates the effect of N2/H2O dilution on a premixed NH3/O2 jet flame in hot coflow under MILD condition. Specifically, the temperature, thermal efficiency, species concentrations, and NOx emissions are analyzed over a wide range of equivalence ratios (φJ). Moreover, fictitious diluents, FN2 and FH2O, are introduced to quantify the physical and chemical effects. The results indicate that the chemical effect of N2 dilution is negligible regardless of φJ. As for H2O dilution, both physical and chemical effects enlarge the volume of the high-temperature region and reduce the temperature peak. In addition, the chemical effect of H2O dilution significantly increases the emissions of unburned NH3, H2, and OH, resulting in a reduction in thermal efficiency by up to 17%. At $\varphi_J \leq 1.0$, replacing N2 with H2O as the diluent reduces the NO emission, but the effect is opposite at $\varphi_J > 1.0$. Notably, the HNO pathway emerges as the most important NO production pathway, being suppressed by H2O dilution at $\varphi_J \leq 1.0$ and enhanced at $\varphi_J > 1.0$. Additionally, the DeNOx pathway dominates the NO consumption and is enhanced by H2O dilution.

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Track14-2 New combustion technologies (2)

Chair: Abhishek Lakshman Pillai
Thursday, May 9; 09:50 - 12:30; Room B

Direct numerical simulation of nanosecond repetitively pulsed discharges for plasma-assisted flame stabilisation in flowing environments

Daniel Fredrich, Stewart Cant
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The plasma-assisted ignition and stabilisation of premixed methane-air flames in moderate to high-velocity bulk flows is investigated using direct numerical simulation. The approach accounts for the primary thermal and kinetic effects of non-equilibrium plasmas sustained by nanosecond repetitively pulsed discharges. The numerical framework is firstly validated against several experimental and numerical test cases from the literature. It is then applied to study the spatiotemporal evolution of the flame kernel ignition and growth in a flowing methane-air mixture with an equivalence ratio of 0.9. For this purpose, a parametric study is performed based on a custom test case at ambient conditions using discrete discharge energies of 2.8 and 3.2 mJ per pulse, pulse repetition frequencies in the range of 20 to 50 kHz, and bulk flow velocities between 0 and 100 m/s. It is shown that the inter-pulse coupling, governed by the relationship between the bulk flow velocity and the pulse repetition frequency, plays a crucial role in the mixture ignition process. Moreover, for a given discharge energy per pulse, a critical discharge kernel convection distance can be determined to distinguish between three different operating regimes: (i) no ignition, (ii) unstable operation, characterised by an oscillating behaviour with periodic flame kernel extinction and re-ignition, and (iii) a stabilised flame. Simulations in three-dimensional space are performed to support the findings and further analyse the dynamics and interaction of consecutive discharge kernels. Finally, the possibility of extending the flame stabilisation limit by means of mixture preheating is demonstrated.

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Efficiency analysis of ignition by Nanosecond Repetitively Pulsed discharges using a low-order approach

Stéphane Q. E. Wang[1], Yacine Bechane[2], Nasser Darabiha[1], Benoît Fiorina[1]
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Plasma-assisted combustion is an interesting method to promote the ignition of a lean reactive mixture instead of conventional spark plugs. Especially, Nanosecond Repetitively Pulsed (NRP) discharges are an energy-efficient way to initiate and control combustion processes. Recent experimental and numerical studies have shown that ignition success or failure results from the competition between the discharge energy accumulation, the gas residence time in the discharge region, and the combustion chemistry. In this work, plasma-assisted ignition is modeled and analyzed by considering a perfectly-stirred reactor whose volume represents the one surrounding the interelectrode region. NRP discharges are applied inside the reactor using a phenomenological model to initiate the combustion of the injected fresh mixture. The approach allows to numerically identify, at a low CPU cost, a plasma-assisted ignition efficiency map in terms of the amount of energy per pulse and the pulse repetition frequency. Moreover, a criterion based on the residence time, inter-pulse time, and chemical time is introduced to predict the successful formation of a reactive kernel.

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Modeling of turbulent flame enhancement by Nanosecond Repetitively Pulsed discharges using a low-order approach

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Plasma-assisted combustion (PAC) is a promising method to stabilize turbulent premixed flames in lean regimes, which are prone to instabilities and extinction. Among the plasma technologies, Nanosecond Repetitively Pulsed (NRP) discharges are an energy-efficient way to enhance and control combustion processes. Recent numerical analyses of a lean bluff-body turbulent premixed methane-air flame have shown that the heat and the radical O produced by NRP discharges mainly induce OH, H$_2$, and O$_2$ through the dissociation of burnt gases. Because of their long lifespans and thanks to the bluff-body recirculating zone, they are advected to the flame front where they are consumed, increasing the chemical

reactivity. Subsequently, the local increase in heat release rate anchors the turbulent flame front, allowing it to develop further downstream and leading to a rise in the total flame surface and power. In this work, PAC is modeled by considering two perfectly-stirred reactors (PSR) and a counterflow premixed flame. Respectively, they represent the interelectrode region, recirculating zone, and flame front. The first PSR employs a phenomenological NRP discharge model, and the second one a temporally evolving inlet. The approach reproduces the mechanisms of turbulent premixed flame stabilization by NRP discharges at a low CPU cost.

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Effect of micro-mixing on nanoparticle production in flame-synthesis: a priori validation of subgrid models for the Batchelor scale

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The optimization of nanoparticle flame synthesis to produce high-quality materials requires a deep understanding of multi-scale interactions between turbulence, flame, and particles. Direct Numerical Simulations (DNS) are classically performed to understand the strong coupling between turbulence, combustion, and aerosol processes. However, the low diffusivity of particles leads to a characteristic Batchelor scale potentially smaller than the Kolmogorov scale. In this context, the aim of this work is:

1) The characterization of micro-mixing effects on particle size and morphology.
2) The a priori evaluation of subgrid models to account for the aerosol processes at the Batchelor scales when using classical DNS grids, where the Kolmogorov scale is resolved but not the Batchelor nanoparticle scale.

A two-mesh strategy was developed: the gas phase is resolved at the Kolmogorov scale, while the particle phase is solved on a finer mesh resolved at the Batchelor scale. An H2/air non-premixed flame interacting with a vortex will be simulated using a monodisperse three-equations model. Different initial conditions for the solid phase and model parameters will be considered to provide insights into the role of micro-mixing on nanoparticle prediction and the capacity of subgrid models to account for them.

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Chemical Evaluation of a Gas Turbine Model Combustor under Diluted and Preheated Conditions Using LES

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Large eddy simulation of a Gas Turbine Model Combustor (GTMC) is performed under both normal and diluted/preheated conditions considering a detailed reduced chemical mechanism through the eddy dissipation concept (EDC) volumetric combustion model. To deliver the same outlet conditions, about 36% reduction in fuel flow rate in addition to 32% dilution of the incoming air (EGR) and an air preheat to 730 K are used in the diluted/preheated case. The accuracy of the present simulations is assessed by comparing the results to the available experimental data. To investigate premixedness, flame indices based on CH4 and CO are evaluated, which shows that far from the inlet nozzle, the CH4 reactions are sustained mostly in premixed mode, while the CO reactions mostly stay in non-premixed mode. Moreover, it is shown that dilution/preheat can lead to higher concentrations of combustion radicals and slow reaction zones at the end of the reactant jet. Finally, slow elementary reactions are shown to have lower sensitivity to the strain rate in the diluted/preheated case, while dropping in high strain regions for the normal operation case, which plays an important role in determining the locations of Formaldehyde formation and heat release.

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Plasma-assisted MILD combustion: Induced velocity effects

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Plasma-assisted combustion has been of great interest in the past years to improve the combustion process against the drawbacks in terms of engine performance, flame stability, fuel consumption, and hydrocarbon pollutants. In recent years, the effect of non-equilibrium plasma has been studied experimentally to understand the dynamic and chemical effects. New observations such as very dilute combustion, cold flames, flameless combustion, and plasma discharge control have been reported. In the works carried out, laboratory tools have often been used to create plasma discharge in the combustion environment and check the mentioned effects. Along with experimental activities, numerical works using different

software in one and two dimensions have been of interest. In these numerical works mostly, the dynamic and thermal effects of plasma are applied as specific parameters in the form of initial and default boundary values. In the present work, unlike the aforementioned works, instead of prejudging the effects of plasma, the dynamic effects of plasma have been modeled using the Suzen-Huang model in a mild combustion environment, and the results have been compared and analyzed with the existing experimental results. It can be seen that the Suzen-Huang model can simulate the dynamic effects of plasma in the combustion environment.

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Unveiling the Impact of Magnetic Fields on Jet Diffusion Flame Flickering

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Gradient magnetic fields have been proven to be an effective approach to modify stability of flames. Observations under a negative gradient field revealed low-frequency oscillations, similar to gravity-induced effects, attributable to Kelvin-Helmholtz instability vortices. The variation of frequency and amplitude has been concluded from experimental observation, but the fluid dynamics behind vortex generation and motion lack detail. This study presents three-dimensional numerical results detailing the temporal and spatial evolution of transitional jet diffusion flame vortices, validated against experimental data. Computational experiments were performed to investigate the effects of initial momentum, volumetric expansion, buoyancy, and gradient magnetic force on the coherence of the vortex structures. Enhanced magnetic fields reduce vortex length, increase generating and shedding frequency, and shift vortex generation position upstream. In this situation, vortices more easily pinch off the flame, and under a strong magnetic field, they may even directly cause blow-out. Due to the relatively low Reynolds number, there are no shear flow vortices generated within the flame surface, minimizing the impact of initial momentum and volumetric expansion. Buoyancy and magnetic forces synergistically influence vortex dynamics, with the role of buoyancy diminishing under stronger magnetic fields. This research elucidates magnetic field-induced flame oscillations and aids in understanding gravity-driven outer vortices, contributing to the in-depth study of flame stability.

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Reaction analysis of frequency dependence on ignition delay time of CH4/Air mixture by repetitive supply of active species

Akira Shioyoke, Jun Hayashi, Hiroshi Kawanabe
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Numerical analysis was conducted to simulate nanosecond pulsed repetitively discharge which is attracting attention as a method for stable flame kernel formation in lean combustion. The effect of pulse repetition frequency on the ignition delay time of CH4/air mixture was investigated using reaction analysis. In this report, methane, the lightest hydrocarbon fuel, was focused and compared with higher hydrocarbons, which can be ignited through Low-Temperature Chemistry (LTC) and H2O2 loops. The nanosecond pulsed discharge was considered as the rapid decomposition of initial chemical species. Zero-dimensional reaction calculations simulating the ignition process through the repeated supply of active chemical species were performed using perfectly stirred reactor model SENKIN. The analysis results, consistent with experimental findings, demonstrated that the ignition delay time is minimized at a specific frequency, indicating the presence of characteristic times in chemical reactions. The difference in reaction pathways between the ignition process driven by the addition of active chemical species and thermal ignition is discussed. Based on the reaction pathway which input active chemical species are consumed, important species and reactions influencing the characteristic time of chemical reactions are discussed. Furthermore, the effect of discharge pulse numbers and input energy on the ignition process is examined.

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Track15 Numerical methods for reacting flows

Track15-1 Numerical methods for reacting flows (1)

Chair: TBD
Wednesday, May 8; 10:40 - 12:20; Room F

Quantum computing of reacting flows via Hamiltonian simulation

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We report the quantum computing of reacting flows by simulating the Hamiltonian dynamics. The scalar transport equation for reacting flows is transformed into a Hamiltonian system, mapping the dissipative and non-Hermitian problem in physical space to a Hermitian one in a higher-dimensional space. Using this approach, we develop the quantum spectral and finite difference methods for simulating reacting flows in periodic and general conditions, respectively. The present quantum computing algorithms offer a "one-shot" solution for a given time without temporal discretization, avoiding iterative quantum state preparation and measurement. We compare computational complexities of the quantum and classical algorithms. The quantum spectral method exhibits exponential acceleration relative to its classical counterpart, and the quantum finite difference method can achieve exponential speedup in high-dimensional problems. The quantum algorithms are validated on quantum computing simulators with the Qiskit package. The validation cases cover one- and two-dimensional reacting flows with a linear source term and periodic or inlet-outlet boundary conditions. The results obtained from the quantum spectral and finite difference methods agree with analytical and classical simulation results. They accurately capture the convection, diffusion, and reaction processes. This demonstrates the potential of quantum computing as an efficient tool for the simulation of reactive flows in combustion.

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Effect of the two-phase flow on the throat erosion feature of the C/C composite nozzle

Zheng Yang, Junwei Li, Wenhao Zhang, Xiang Li, Ningfei Wang
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For the solid rocket motor C/C composite nozzle, a two-phase flow calculation model was developed to simulate the erosion process, obtain the rate of change of the erosion rate, and analyze the change of the flow field in the erosion regime. Calculation results show that the nozzle convergence section and the throat are affected by particle erosion and thermochemical ablation, while the nozzle divergent section is only affected by thermochemical ablation, the average thermochemical ablation rate of the nozzle throat is 0.0420mm/s, and the ablation of the throat leads to the reduction of the gas flow rate, which decreases the performance of the engine. Finally, the simulation calculations were validated by erosion tests, which yielded an average thermochemical ablation rate of 0.0432 mm/s for the throat measured in the test data and an error of 2.8 percent for the simulation calculations, indicating a good agreement between the two.

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Simulation methodology for cryogenic liquid hydrogen leakage, dispersion prediction and risk assessment

Leons Antony Lawrence, Sourabh Shrivastava, Vivek Kumar, Pravin Nakod
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As the world is shifting to Hydrogen based energy solutions, there is an increasing need to develop safe modes of storage and transportation of Hydrogen. Currently Hydrogen is stored and transported in cryogenic liquid state due to the high energy density that it offers. There is a pressing need to understand the behavior of such systems in case of an accidental leak. In this work we would like to present a simulation methodology to predict cryogenic hydrogen leakage, dispersion into the atmosphere and the flammability risk associated with it.

A high fidelity and a low fidelity method is proposed.

- High fidelity model involves detailed two-phase modeling with real gas properties of Hydrogen, expansion of the supersonic jet, and the corresponding phase change that happens when cryogenic hydrogen mixes with air.
- Low fidelity model : A notional nozzle based approach was evaluated. It is based on partially expanded single phase gaseous hydrogen, with real gas properties. It is very quick and easy model to evaluate different design concepts.

The concentration of hydrogen along the jet axis was evaluated for both the methods and compared with published test data.

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A large scale H2-CH4 industrial furnace Lattice-Boltzmann study taking into account Radiation Heat Transfer

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Recent developments on Lattice Boltzmann Method (LBM) have established this approach as an alternative to traditional CFD methods for combustion applications. However, application to industrial burners remains challenging due to the large range of scales involved, and the geometry complexity. In this study, we present large-eddy simulations of a partially premixed H2-CH4-air industrial burner using a hybrid Lattice-Boltzmann method. Due to the considerable length of the 6-meters furnace and the burnt gases content, radiative heat transfer is here fundamental, and taken into account for the first time in this framework. To couple Lattice-Boltzmann modelling of reacting flows and radiative heat transfer, the spherical harmonics method of first order is adopted (P1 approximation). This method transforms the radiative transfer equation into a set of coupled partial differential equations (PDEs). The Weighted-Sum-of-Gray-Gases approach (WSSG) is used to represent the spectral dependence of radiative properties. The primary objective of this work is to study the influence of the H2-CH4 fuel blend composition on the burner characteristics, ranging from pure methane to pure H2. Through our numerical simulations, we examine the fuel composition impact on flame behaviour, temperature distribution, and pollutant formation. To validate our simulations, the numerical results will be compared with experimental data.

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Track15-2 Numerical methods for reacting flows (2)

Chair: TBD
Wednesday, May 8; 13:30 - 15:10; Room F

Effect of Two-Strut Parallel-Fuel Injection Scheme on Mode Transition in Scramjet Combustor

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Mode transition in a two-strut dual-mode Scramjet combustor is tested numerically. Results are compared with mode transitions in a single-strut, dual-mode Scramjet combustor based on the German DLR configuration. The two-strut configuration allows the manipulation of two important flow parameters responsible for mode transition. Firstly, it allows fine-tuning the location of the primary heat release zone between the two struts. Secondly, it allows manipulating the cross-sectional area of the supersonic air stream in the vicinity of this primary heat release zone. Since the tendency of a supersonic air stream to choke thermally is influenced by both heat addition and cross-sectional area variation, the dual-strut configuration might provide a way to delay mode transition in a dual-mode scramjet combustor.

Numerical simulations using the commercially available ANSYS-FLUENT software running on an HPC platform are used to simulate the influence of a dual-strut configuration on heat release and flow cross-section variation. Two-dimensional, steady-state, k-ω, density-based implicit solver is used to solve the partial differential equations of fluid flow.

Results suggest that both the cross-sectional area of the outer supersonic flow fields and the location of heat addition to it can be altered by altering their position and size and orientation of the two struts, a behaviour which will be investigated in detail in this study. Effect of such variations on the propensity of supersonic combustors to undergo Sudden mode transitions will be reported.

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Mesoscale modeling on the melt layer of metalized propellants with surface stress evolution

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While progress has been made in the modeling of burning surface of solid propellants, the intricate interactions within the melt layer involving three distinct phases and multi-materials remain unresolved and present a formidable challenge. This study aims to present a comprehensive analysis on the combustion characteristics of metal-added propellants that considers reactive metal particles of random size. Three pivotal techniques are developed for 1) tracking the dynamics of two-phase interface with deforming material boundaries between reactive particle and binder, 2) incorporating the full stress field evolution within each particle, and 3) introducing the phase and composition identifiers to monitor the process of reaction via oxide cap formation, heat transfer between multi-materials, and agglomeration of metal oxide. The results on the pressure, temperature, stress, and material phase reveal the emergence and expansion of the melt layer, which includes isolated solid reactants with a multi-phase oxide cap and vaporized binder separated from the unburnt region. The quantitative weight fraction analysis provides insights on the three distinct sections, demarcated by predominant shifts in the material phases. The simulation successfully replicates the visual images taken from the experiments without the need for introducing phenomenological models.

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Simulations of hydrogen-air detonations using DSMC

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Molecular level simulations of one-dimensional (1-D) hydrogen-air detonations are performed using the Direct Simulation Monte Carlo (DSMC) method. DSMC emulates the motion of real molecules and can solve molecular transport processes, internal energy relaxation, and chemical reactions directly through molecular collisions. It is a robust tool for fundamental studies of reacting flows under thermal and chemical non-equilibrium. Hydrogen flames have been successfully simulated with DSMC by using both the TCE model, with uses the traditional Arrhenius based reaction rates, and a QK model, which makes direct use of collision data for computing reaction probabilities. In this analysis, TCE model is employed for simulating 1D detonations. Two cases of stoichiometric hydrogen-air mixtures are considered. A preheated case at an initial temperature equal to 900 K and an initial pressure of 0.3 atm is simulated first. This is followed by a second case at standard 300 K and 1 atm. The results are compared with the Zel'dovich-von Neumann-Döring (ZND) solution obtained from the Shock and Detonation toolbox.

The preheated case results in a robust and steady detonation structure. The DSMC results for temperature, pressure, flow velocity, density and species mass fractions for this case show excellent agreement with the ZND solution. The case at standard conditions results in a fluctuating induction zone, and DSMC captures these fluctuations effectively but the 1-D profiles differ slightly from the ZND solution. These differences are attributed to the shortcomings in the recombination reaction rate modelling which have received little attention in DSMC. Robust simulations under non-equilibrium conditions will require ab-initio molecular data from Quasi-classical trajectory calculations to provide collision cross-sections for relaxation and reaction rates.

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Fast geometric integration for chemistry

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Fast integration of stiff chemical source terms is a critical requirement for improving the computational efficiency of reacting flow solvers. Geometric integrators based on Lie group methods are a robust solution to maintain the structural attributes of differential equations, including conservation laws and symmetries. This results in simulations that are both more stable and accurate. The approach casts the chemical source term in a generalize Hamiltonian form, which exposes the symplectic nature of the tangent bundle. The evolution of the system is split into two components, namely elongation and rotation, which allows Strang-type splitting to be used. The elongation tensor is efficiently integrated using a second-order Runge-Kutta scheme and the rotation tensor, satisfying the Special Orthogonal Lie group properties, is integrated using a second-order Munthe-Kaas-Runge-Kutta scheme. This technique allows for significantly larger time steps than explicit schemes, while maintaining the accuracy of implicit schemes.Performance evaluations across hydrogen/air, ammonia/air, and RP2/air mixtures demonstrated a speedup of 5-25 compared to traditional stiff integration schemes, highlighting the efficiency and performance of the new approach.

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Track15-3 Numerical methods for reacting flows (3)

Chair: Raja Banerjee
Wednesday, May 8; 15:30 - 17:10; Room F

Comparative study to asses combustion models for pure hydrogen bluff body stabilized flame

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Carbon-based fuels pose a significant environmental threat as their combustion releases substantial amounts of carbon dioxide and other pollutants. This contributes to global warming, extreme weather events, ocean acidification, and air quality degradation. The continued reliance on these fuels exacerbates the climate crisis, with far-reaching consequences for ecosystems and human well-being. Due to its clean combustion characteristics, hydrogen fuel and hydrogen-blended fuels are gaining attention as substitutes for carbon-based fuels.

Designing new combustion systems for industrial applications with high hydrogen content requires a detailed understanding of flame characteristics. This can be derived by studying flame from simplified concept-level configurations with well-defined boundary conditions and utilizing that information as a base to design more complex systems. Computational Fluid Dynamics (CFD) simulations provide detailed insights into the combustion process and can help integrate and test the information derived from concept-level designs to final designs. For conventional hydrocarbon-based combustion systems, the simulation methodologies are well established. However, CFD methodologies for hydrogen and hydrogen blended fuels are still being evaluated and developed by different research groups.

To identify the limitations of standard combustion models and the correct simulation strategy for pure hydrogen bluff body stabilized flame, a series of simulation studies were performed, and conclusions are reported in this paper. Models considered for this study are the detailed chemistry finite rate model (FR), Flamelet Generated Manifold Model (FGM), and Thickened Flame Model (TFM), along with the combinations of Reynolds Average Navier Stokes Model (RANS) and Large Eddy Simulation (LES) turbulence models.

The experimental data used for reference are taken from NTNU's dataset for the turbulent bluff body stabilized flame produced by a lean, fully premixed air/hydrogen. Bluff body stabilized flames are one of the most studied configurations due to their similarities with many combustion systems, enabling detailed study of turbulence-chemistry interactions. The geometry consists of the plenum from where the premix enters and expands for flow conditioning, the injector where the mixture is compressed, and a conical bluff body at the end of the injector pipe to generate a recirculation zone where the flame can stabilize in the shear layers.

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Scale similarity models for filtered reaction rates

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One of the long-standing challenges in large eddy simulation of reacting flow is the modelling of the unclosed chemical reaction rate terms. Here, we explore scale similarity models (SSM) using some new formulations and generalizations. In the few prior studies of SSM for reaction rates found in the literature, the rate is decomposed into the perfectly stirred reactor (PSR) rate plus a residual to be determined by scale similarity. Here, we also explore the alternative decomposition into the PSR rate multiplied by one or more correction factors that are determined by one or more applications of scale similarity. The accuracy of different formulations are compared for laminar and turbulent premixed flames and laminar counterflow flames. Sensitivity to fuel is also investigated by comparing methane, ethene, methanol and hydrogen. Results show that both formulations (added residual or scaling factor) are viable and can perform better than PSR, and multiple levels of SSM can improve the results. Scale similarity appears to be most suitable for fine grids. No clear dependence on fuel or combustion mode was found. Most of the error in the modelled rates pertain to very few reactions whose reactants are artificially brought together by the filter operator.

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A reduced order numerical model for high-pressure hydrogen leak self-ignition

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The numerical study of ignition risk in the case of high-pressure hydrogen leakage contains numerous

challenges. The first is to properly resolve the complex multi-dimensional flow (hemi-spherically expanding shock and contact discontinuity). The second is to properly resolve the diffusion/reaction interface, which has a very small length scale compared to the jet radius [1].

We propose a low-order numerical model for such flows by first decoupling the flow and the diffusion/reaction interface into one cold flow and one reaction interface problem. The flow simulation can be further simplified by assuming the flow in the ambient air is almost axisymmetrical (for a two-dimensional test case) or spherical, which means that the flow only needs one space dimension to be solved. Meanwhile, the diffusion interface is solved with a different space variable to optimize the mesh and use the flow results as boundary conditions. The interface problem is further simplified by using the passive scalar approach recently developed for hydrogen ignition prediction [2].

Both the flow and the interface solver are validated with simple test cases and full configuration results are compared to complete multidimensional simulations.

[1] : A.E. Smygalina, A.D. Kiverin, Self-ignition of hydrogen jet due to interaction with obstacle in the obstructed space. Int. J. Hydrog. Energy, 47 (2022).
[2] : M. Le Boursicaud et al, An improved passive scalar model for hydrogen hazardous ignition prediction, Combust. Flame, 256 (2023).

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A MODAL DECOMPOSITION-BASED PARTIALLY STIRRED REACTOR MODEL FOR TURBULENT COMBUSTION CLOSURE: AN A POSTERIORY STUDY

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Accurately characterizing reactive environments in combustion is crucial for optimizing efficiency and managing emissions. Turbulent conditions in practical combustion systems necessitate a trade-off between computational cost and accuracy, often addressed through Large Eddy Simulations or Reynolds Averaged Navier-Stokes. Closures for the unresolved reaction source terms involve reducing the scalar transport equations to representative variables or direct solving for all chemical species and physical models.

The Partially Stirred Reactor (PaSR) model divides computational cells into reactive and non-reactive parts, showing promise in various combustion regimes. However, accurately estimating characteristic timescales remains a challenge due to their variability within reactive environments. The uniqueness of the cell reacting fraction has also been found to be sub-optimal [1].

Quadarella et al. [2] proposed a modal decomposition-based PaSR model (mPaSR) by means of the computational singular perturbation theory, which relates characteristic time scales for chemistry with the eigenvalues of the Jacobian matrix of the chemical source terms [3]. Although strongly deviating from the original PaSR formulation, abandoning the fine structures concept, a priori results demonstrated the benefits of accounting for multiple reacting fractions. This work presents an a posteriori investigation of the mPaSR model via unsteady simulations of flames exhibiting processes with distinctive time scales.

[1] Péquin, A., et al., Physics of Fluids, 2022.
[2] Quadarella, E., et al., Proceedings of the Combustion Institute, 2022.
[3] Malpica Galassi, R., et al., Combustion and Flame, 2018.

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Track15-4 Numerical methods for reacting flows (4)

Chair: TBD
Friday, May 10; 09:50 - 11:50; Room F

Dual-scale flamelet tabulation using the multi-gate mixture of experts

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High-dimensional flamelet chemtables are required for describing multiple physics in turbulent combustion. Representing the flamelet library using artificial neural networks (ANN) can significantly reduce memory consumption. However, it is difficult to fit all the variables accurately based on the simple feedforward neural network (FNN) model due to the multi-scale distributions of thermochemical variables. To accurately and efficiently represent the multi-scale quantities, we develop a dual-scale tabulation strategy that combines the multi-gate mixture of experts (MMoE) and flamelet/progress variable (FPV) model. In this strategy, two progress variables are defined to represent the time-scale effect. One is the traditional progress variable defined by major products for representing the mapping of small time-scale variables (e.g.,

main species), while the other is an additional progress variable defined by minor species for representing the mapping of large time-scale variables (e.g., NO and PAHs). The proposed tabulation approach is validated by comparing the predictions with those of the FNN tabulation method and detailed chemistry in the a priori manner. The results show that the proposed tabulation approach can better reproduce the detailed chemistry predictions than the FNN method.

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On the impact of scalar boundedness in high-order LES of a nonpremixed jet flame

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We carried out large-eddy simulations (LES) of a three-dimensional temporally evolving turbulent nonpremixed jet flame to evaluate the impact of numerical errors from high-order numerical schemes to discretise convective terms. We focus on the effects of numerical oscillations and scalar unboundedness and compare a newly proposed scheme against an ad hoc remedy to enforce scalar boundedness in LES of nonpremixed flames. Such numerical issues are commonly encountered in under-resolved simulations like LES, especially when using high-order schemes, but their impact is rarely reported. The research compares two high-order numerical schemes in LES against direct numerical simulation data. The first, a high-order central-difference scheme with compact filtering, generates significant numerical oscillations at under-resolved scalar interfaces and subsequent mass fraction excursions, resulting in an unstable simulation. Ad hoc trimming of such excursions stabilises the simulation, but residual oscillations contaminate radicals and heat release rate solutions. These inaccuracies accumulate over time and cause non-physical changes in chemical reactions, leading to pronounced deviations in radical mass fractions and reignition flame temperature. In contrast, a newly proposed high-order bounded scheme avoids these spurious oscillations and maintains mass fraction boundedness, yielding a stable LES and improved accuracy in flame reignition predictions. These observations demonstrate the detrimental effects of numerical oscillations, mass fraction excursions, and trimming on LES stability and predictive accuracy. A comparison with other LES in the literature also suggests that the influence of numerical schemes is comparable to that of combustion models, highlighting the importance of using accurate high-order schemes in turbulent flame LES.

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Modelling of Turbulent Non-premixed Blend of NH3/H2/CH4 in a Jet Flame Using Flamelet Model

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Hydrogen is emerging as a promising solution to mitigate the adverse environmental impacts of fossil fuels. However, the practical challenges related to its storage and transportation and the possibility of hydrogen embrittlement have presented significant challenges. Ammonia (NH3) is being actively considered as an alternative carbon neutral fuel. However, its low calorific value and low flame speed are some of the challenges that needs to be addressed before it can be widely used in combustion applications. In this work, a semi-detailed NH3/H2/CH4/n-C12H26 mechanism consisting of 242 species and 1769 reactions including both nitrogen oxides (NOx) and soot sub-mechanisms have been used to simulate combustion in a jet flame. As ammonia has a poor laminar flame speed, blending it with methane and hydrogen will significantly improve its flame speed. The effect of NH3-H2-CH4 composition on emission of NOx, soot and unburnt NH3 is investigated at various ambient pressures. Additionally, the effect of ambient pressure on total greenhouse gas emission that includes the sum total of CO2 and N2O is investigated because production of N2O, which has a very high greenhouse gas index, will be favored at elevated pressures.

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Large-Eddy Simulation of Nanoparticle Synthesis in Turbulent Spray Flames Using a Lagrangian FDF Approach with Different Mixing Models

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Flames, providing stable thermal conditions, are the prevalent choice for nanoparticle formation, establishing flame-based methods as the standard in nanoparticle production. While nanoparticle synthesis at the laboratory scale typically exhibits laminar characteristics with moderate Reynolds numbers and low pressure, replicating these conditions in pilot-scale operations is challenging, and turbulent flows are anticipated. The resultant nanoparticles are influenced not only by coagulation and sintering but also by the impact of turbulence on local particle number concentration and morphology.

In the present study, the Lagrangian filtered probability

density function (FDF) method within large eddy simulation (LES) is employed to model iron oxide nanoparticle synthesis in the spray flames. In the transported FDF approach, no model is required for the source term of each nanoparticle section, while the conditional subgrid diffusion effect needs closure through a turbulent mixing model. Two classical mixing models, IEM (Interaction by Exchange with the Mean) and modified Curl, are tested. Additionally, an advanced approach, the Euclidean Minimum Spanning Tree (EMST) mixing model, is implemented to assess the impact of localness in composition space. A comparison of the three mixing models against measurements will be presented at the conference.

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Robust dynamic stencil construction for high-order Adaptive Mesh Refinement in Direct Numerical Simulation of combustion

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Adaptive Mesh Refinement (AMR) provides the ability to ensure that mesh resolution is always sufficient in regions of the computational domain where the solution is varying most strongly. This is especially important in Direct Numerical Simulation (DNS) of combustion where high accuracy is essential and flames are often thin. High-order spatial reconstruction schemes based on a finite-volume approach offer high accuracy together with good conservation properties on the locally-adapted mesh. Such schemes require fairly large and well-configured stencils to ensure accuracy and stability of the solution.

An algorithm has been developed that uses Singular Value Decomposition of the spatial solution-reconstruction matrix to guide the construction of stencils on-the-fly while guaranteeing the stability of the solution. The algorithm has been implemented in the combustion DNS code HAMISH which uses a fourth-order spatial reconstruction scheme with pointwise AMR, together with third-order adaptive Runge-Kutta time-stepping. Results have been obtained for a range of combustion test cases that demonstrate the effectiveness and robustness of the approach.

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Track15-5 Numerical methods for reacting flows (5)

Chair: TBD
Friday, May 10; 13:00 - 15:00; Room F

A high-order compressible Eulerian stochastic fields solver based on AMReX

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This work introduces a high-order compressible Eulerian stochastic fields solver built on the AMReX software framework, offering a robust and versatile platform for simulating turbulent reacting flows across all Mach numbers. While the probability density function model has a successful track record of modelling turbulence-chemistry interactions, implementation using the Eulerian stochastic fields approach eliminates the need for coupling between Lagrangian and grid-based solvers. The present implementation uses a fully coupled joint velocity-scalar-energy formulation, allowing closures of non-linear chemical source terms and non-ideal equations of state. The model does not require LES-type closures and can adapt the mesh to satisfy predefined resolved energy criteria. The solver integrates many of AMReX's capabilities, including adaptive mesh refinement and portability across various CPU/GPU architectures. Complex geometries are supported using the embedded boundary method or a novel immersed boundary method. The core solver centres around a 5th-order WENO/TENO reconstruction while chemical reaction is powered by the PelePhysics library, supporting arbitrary detailed chemical mechanisms, and direct or matrix-free implicit integration. The code demonstrates its effectiveness in accurately modelling turbulent reacting and non-reacting flows through standard benchmark cases as well as challenging scenarios such as supersonic combustion. Verification of the numerical methods and turbulence model will be presented.

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Bayesian optimization of in-situ adaptive tabulation for marine diesel engine CFD simulations

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This study presents a comprehensive optimization study of In-situ Adaptive Tabulation (ISAT) control param-

eters, in the context of enhancing the computational efficiency of reactive marine diesel engine simulations using computational fluid dynamics (CFD). The methodology integrates a multi-objective Bayesian optimization framework with the OpenFOAM CFD solver, enabling efficient exploration of the ISAT parameter space. Standard Gaussian process surrogate models were combined with state-of-the-art acquisition functions, facilitating the discovery of optimal configurations balancing the trade-offs between simulation accuracy and computational reduction. The optimization campaign was conducted using a series of high-fidelity 3D CFD simulations of a Wärtsilä 20 marine diesel engine under diesel combustion conditions. The simulations incorporated detailed chemistry, a moving computational mesh, and diesel surrogate fuel injection. The results highlight the criticality of rigorously choosing ISAT's configuration parameters. Poor configurations were shown to crash and stall simulations, resulting in a net-negative effect on computational efficiency. Despite this, a wide range of computational reduction was shown to be possible, with varying effects on simulation accuracy. Finally, guidelines are provided for effective parameter selection in ISAT configurations.

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Adjoint-based numerical and experimental data assimilation for shock-tube ignition delay predictions

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Simulations of shock-driven ignition delay are crucial to the design of airbreathing detonation-based combustors. High sensitivity to kinetic model parameters yields high uncertainty of numerical calculations relative to experiments, particularly when detailed kinetic models are applied far from the conditions used to calibrate the elementary reactions. We present an application of solver-coupled data assimilation to shock-driven ignition delay time (IDT) predictions. The optimization method solves the adjoint flow equations to calibrate semi-global kinetic model parameters and additional corrective terms. Target data are the flow fields obtained from detailed-chemistry calculations and experimental pressure and temperature probes. Predictions for in- and out-of-sample conditions are shown.

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Development of a New Library in OpenFOAM for Simulations of Reacting Flows with Surface Reactions

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Recently, hydrogen (H2) production has gained significant attention since H2 has emerged as an effective and clean alternative to fossil fuels, especially in the power generation sector, to meet carbon neutrality by 2050. While many experimental studies on the H2 production from catalytic ammonia (NH3) decomposition have been conducted, the numerical investigation on this field is limited due to lacking sufficient computational fluid dynamics (CFD) package for public use to handle surface reactions occurring in catalytic processes. In that context, we developed a new surface chemistry library in OpenFOAM (OF) platform, a free and robust open-source CFD package, to provide a sufficient CFD tool for researchers working on this field and combustion community since there is no such library officially available in OF. The developed library can handle several types of typical surface reaction rate models consisting of the basic Arrheninus form, sticking coefficient, and surface coverage dependence models. It was validated against experimental data and previous studies by performing two dimensional (2-D) simulations of fixed packed-bed catalytic reactors. The results showed a good agreement between predicted and benchmark data, implying that our implementation is proper, and our developed library can be used for simulations of catalytic processes with the utilizations of detailed micro chemical kinetic models.

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Explicit filtering LES of turbulent lifted jet flames with a multi-regime combustion model

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Computations of turbulent lifted jet diffusion flames are performed using explicit filtering large eddy simulations (EFLES). LES solutions are obtained by solving species transport equations using reduced chemical mechanisms. A dynamically adapted spatial low pass filter is used limit flame generated gradients in flow field variables to values that can be resolved by the LES mesh. A flame front broadening factor is used to scale chemical source terms to ensure the recovery of nominal 1D premixed flame

speed on resolution of the LES mesh. In a lifted jet flame, oxygen from the co-flow stream diffuses into the core jet flow ahead of the flame attachment point. This leads to flow regions with both premixed and non-premixed combustion regimes. Therefore, a combustion regime sensor based on the angle between mixture fraction and progress variable gradients is used to detect premixed and non-premixed combustion regions and adjust the flame front broadening factor appropriately based on how the relevant flame length scales compare with the local grid size. We will compare DNS/experimental results for lifted hydrogen and ethylene jet flames with LES solutions for flame lift-off height, flame brush structure etc. in the final work.

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Track15-6 Numerical methods for reacting flows (6)

Chair: Ville Vuorinen
Friday, May 10; 15:20 - 17:00; Room F

Numerical Analysis of Hydrogen Microjet Flames

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Microburners are of interest because of their wide application potential in engines, power efficient heat sources, compact thermovoltaic converters of energy and further devices. The main element of such burners is the micronozzle supplying the burnable gas. When the latter does not contain oxygen, but mixes with air after the injection, a micro-diffusion flame results, which precludes any danger of flashback. Hydrogen occupies a central role for clean and efficient energy supply. The scope of the present work is the numerical analysis of diffusion flames of high-speed hydrogen microjets.

Microjet diffusion flames of hydrogen were investigated experimentally by Kozlov et al. [1,2] and Shmakov et al. [3]. In those experiments, a quite interesting flame topology was observed, which was named as “bottleneck flame”. Here, depending on the injection conditions, a compact spherical/ellipsoidal flame in the burner nearfield was formed that was followed by rather customary free-jet like topology.

To the best of the author’s knowledge, such flames have so far not been investigated computationally. Thus, the purpose of the present study is the numerical analysis of such flames, to see if the measured flame patterns can be predicted with sufficient accuracy. There are many modelling challenges. Due to the very small injection diameter, the jets are laminar at the injection but turbulence can develop in the free shear layers, which is challenging for turbulence modelling. The sound speeds in hydrogen and air differ by a factor about four. This leads to a rapid variation of the local Mach number in the mixing zone, which can be challenging with respect to compressibility for the present high-speed jets. The comparably high diffusion coefficient of hydrogen with respect to the remaining species is a further challenge for combustion modelling.

Different turbulence models as well as different combustion models utilizing global and detailed reaction mechanisms will be applied and validated based on the available measurements.

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Application of a reduced chemical mechanism for combustion in vitiated air conditions in RANS simulations

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In order to better take into account the effects of vitiated air in combustion processes in an after-burner, a new reduced chemical mechanism called 2S_KERO_M2 [1] has been implemented for reacting transported species RANS simulations. It consists of two reactions and six transported species (kerosene, O2, N2, CO2, CO, H2O), in which the pre-exponential constants are adjusted to match premixed flame speeds in rich conditions. The pre-exponential constants depend on both the local equivalence ratio and the equivalence ratio in the oxidizer stream characterizing the reheat conditions. The implementation of the scheme is validated against semi-detailed chemistry in 1D laminar flames for several values of the pre-burner equivalence ratio. The methodology is then applied to a semi-industrial practical case [2], representing a bluff-body stabilized flame in vitiated air. Simulations are based on the k-epsilon model and the Eddy-Dissipation Concept for turbulence/combustion interactions. Liquid spray injections are modeled using the lagrangian framework. Heat release and equivalence ratio fields are compared to mean experimental data and LES computations and show good agreement with regards to flame shape and position

at different levels of vitiation.

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[2] Cross, Caleb, et al. "Determination of equivalence ratio and oscillatory heat release distributions in non-premixed bluff body-stabilized flames using chemiluminescence imaging." Turbo Expo: Power for Land, Sea, and Air. Vol. 54624. 2011.

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Acceleration of multidimensional simulations with detailed kinetics via Chemistry Agglomeration

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In this work, we present a numerical technique based on the concept of Chemistry Agglomeration [1] to accelerate the integration of the chemical step in the context of operator-splitting methods. The proposed technique consists in splitting on-the-fly the kinetic mechanism into clusters (or sub-mechanisms) with a smaller number of species via a partition/clustering algorithm. Once the clusters of species have been identified, the integration of the chemical step, instead to be carried out on the complete kinetic mechanism, is split into a number of sub-steps equal to the number of identified clusters. Since the cost of chemistry integration increases more than quadratically with the number of species, solving a sequence of smaller sub-mechanisms is computationally less expensive than directly solving the entire mechanism.

Two benchmark cases have been considered: i) a laminar, pulsating laminar coflow diffusion flame fueled by a mixture of C2H4 and N2; ii) a 2D, turbulent, non-premixed flame burning n-C7H16 subject to decaying isotropic turbulence. In both cases, a detailed kinetic mechanism accounting for the formation of soot particles and aggregates was considered. The results are promising, showing both accuracy and computational efficiency, demonstrating the potential of the methodology for multidimensional CFD simulations of reactive flows with complex chemistry.

References

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Effects of radiation- and combustor-wall boundary condition on LES of turbulent combustion

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Numerical simulations of turbulent combustion is challenging due to the combined complexities of turbulent flow and combustion chemistry. High fidelity simulation models such as Large Eddy Simulations (LES) with finite rate chemistry effects and small detailed reaction mechanisms, whereby the combustion chemistry is explicitly solved for, have in spite of its high cost, provided increased understanding and predictive capabilities. Two aspects of such simulations that often are neglected because of their added complexity and information deficit are thermal radiation and the influence of the thermal combustor wall boundary conditions. Thermal radiation can be included in combustion simulations using models such as the P1 or Discrete Ordinates (DO) models but additional terms due to the filtering in LES occur and must be treated. Information regarding the actual benefits of radiation modeling is scares, and here we aim to provide qualitative and quantitative data for a few selected swirl- and bluff-body- stabilized flames for which experimental data is available. For confined turbulent flames the issue of thermal combustor wall boundary conditions is equally or even more important. Due to lack of information from experiments it is challenging to infer sufficiently accurate thermal boundary conditions. Here, we will investigate the sensitivity to different combustor wall boundary conditions and their effects of the turbulent flame and its dynamics.

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Track17 High-performance computing for combustion applications

Track17-1 High-performance computing for combustion applications (1)

Chair: TBD
Wednesday, May 8; 10:40 - 12:20; Room H

Simulation of low-temperature plasma ignition of ethylene/air mixtures at scramjet cavity conditions with high-fidelity models for non-equilibrium plasma discharge, acoustic and vibrational relaxation, hydrodynamic mixing, and mixture ignition

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A comprehensive framework based on the AMReX library and associated reactive flow solvers is assembled to simulate the ignition of ethylene/air mixtures at 0.5 atm and 600 K, corresponding to conditions in the cavity of scramjets. The modeling framework features a plasma solver capable of simulating streamer propagation and energy deposition over time scales of 100 ns using chemical plasma fluid models and physics-based closures. Following isochoric energy, which creates a large population of molecules in electronic and vibrational non-equilibrium, the reactive compressible flow solver PeleC is used to simulate the outward propagation of shock waves during the expansion of hot gases in the plasma channel up to 10-50 us. Next, the solver PeleLMeX integrates the low-Mach restriction of the Navier-Stokes equations for up to 1-10 ms, capturing the ignition of a flame kernel. The framework is computationally efficient, enabling the simulation of multiple nanosecond voltage pulses at practical repetition frequencies with high-fidelity models void of common simplifying assumptions used in previous work. Based on our large-scale simulations, a complex interplay between energy deposition, hydrodynamic mixing, and ignition emerges, whereby the first-principles simulation of plasma discharges over multiple pulses is key to representing subsequent mixing and ignition accurately.

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The Effect of Combustion-Induced Instabilities on Shock-trains in a Scramjet Isolator

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The isolator plays a vital role in the operation of a scramjet engine, providing air compression through a sequence of shocks known as the 'shock-train'. The development of the boundary layer along the isolator wall and the instabilities due to the combustion downstream of the isolator are known to affect the shock-train dynamics and, consequently, the overall performance of the scramjet. This study investigates this complex dynamics of shock-trains using Embedded-boundary (EB) method and adaptive mesh refinement (AMR). The main goal is to understand how combustion instabilities downstream of the isolator affect the shock-train dynamics. The computational model is axisymmetric and includes a cavity combustor downstream of the isolator. Ethylene is used for the fuel which is injected to the air upstream of the combustor. The EB method is used for modeling the geometry which avoids the need for a complex geometry-conforming mesh whereas AMR provides finer grid resolution in the regions of interest keeping the computational cost tangible. A precursor simulation is used for generating turbulent inflow conditions which allows to study the interplay between combustion and shock-trains for various inflow conditions. The results of shock-train behavior with and without combustion are discussed.

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GPU-based DNS enables dissection of cracking, turbulent mixing, and oxidation processes in NH3/H2 jet flames

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Ammonia-hydrogen blends will play a pivotal role for future carbon-free combustion systems. To minimize remaining emissions in ammonia combustion, staged combustion systems, such as rich-quench-lean technologies, are proposed. However, the combustion behavior of turbulent rich ammonia-hydrogen mixtures lack comprehensive understanding. In particular, the quantification of complex phenomena like partial cracking, hydrogen slip, and post-flame stratification and their interaction with flame structures and pollutant formation remains insufficient.

This is a major scientific barrier hindering the realization of NH3/H2 blends for carbon-free combustion. Recent HPC advancements, particularly in GPU-based systems, enable combustion DNS beyond academic configurations.

Utilizing nekCRF, a new GPU-based spectral element solver based on nekRS, we perform finite-rate chemistry DNS of a rich, turbulent premixed jet flame. This unique data set provides fundamental insights into the intricate interaction of reactions and turbulence that are crucial for developing future models. The analysis focuses on NH3/H2 interaction, revealing residual H2, minimized NH3 slip, and enhanced heat release through turbulent mixing. By leveraging GPU acceleration and employing a novel spectral element solver, this research not only advances our understanding of ammonia combustion but also showcases a paradigm shift in computational efficiency, offering a promising avenue for developing sustainable energy solutions.

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Fuel-specific code generation for thermochemistry and transport properties for CPU- and GPU-based solvers

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The transition to green energy requires the adaptation of combustion applications to carbon-free fuels such as hydrogen and ammonia. Achieving this objective is not possible without highly accurate direct numerical simulations (DNS) to elucidate the complex physical phenomena. In turbulent combustion DNS, a significant fraction of the total simulation time is spent on the evaluation of chemical source terms, thermodynamic properties and transport coefficients. In this work, we present a software package that automatically generates efficient fuel-specific kernels for these quantities. The starting point is a Cantera yaml file containing the reaction mechanism and the data required for the calculation of the thermodynamic and transport properties, which is processed to generate the fuel-specific kernels. Different strategies are used to optimize the kernels for CPUs and GPUs, with the latter being further optimized for the respective GPU architecture. The accuracy of the generated kernels is automatically checked against reference values for species production rates, thermodynamic properties and transport coefficients calculated using Cantera and stored for comparison. The kernels' performance is evaluated on the latest CPU and GPU architectures from Nvidia, AMD and Intel.

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Track17-2 High-performance computing for combustion applications (2)

Chair: TBD
Wednesday, May 8; 13:30 - 15:10; Room H

Multistep high-order time adaptive coupling of black-box solvers for multiphysics simulations

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Multiphysics simulations are paramount in many applications and often occur through the coupling of various physics in different physical domains coupled through lower-dimensional surfaces. Relying on code heritage, it is desirable to design a coupling strategy that allows to reuse existing model-specific solvers with minimal modifications. However, in most existing numerical coupling strategies, the design of such strategy comes with low-order accuracy in time and difficulties with regard to controlling the errors related to the coupling strategy. In this contribution, we introduce a novel strategy that ensures adaptive, accurate and stable coupled simulations. The principle is a multistep coupling scheme, which relies on the history of the exchanged quantities to enable a high-order accurate coupling with time adaptation and error control. Explicit and implicit variants are discussed.

Numerical experiments conducted with an open-source demonstrator on a conjugate heat transfer problem show that high-order convergence can be reached, and that stability is favourable compared to other classical approaches. We propose some insight on the numerical analysis of the proposed strategy, and extensions to simulations in combustion as well as the case of volume coupling are discussed.

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AATE: Advanced Analysis Tool for Engines

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In this study, we introduce an open-source platform for simulation, analysis, and post-processing of internal combustion engines (ICE) in the OpenFOAM framework–AATE ((/ˈɑːteɪ/), the Advanced Analysis Tool for Engines. We introduce a set of developments that enables the user to achieve full-cycle engine simulations within OpenFOAM. The developments consist of a new, robust and flexible mesh deformation method which is seamlessly coupled with run-time MPI-parallelised volume mesh-to-mesh mapping and arbitrary non-conformal sliding interface techniques. To ensure consistency, efficiency, and extensibility, the implementation is carried out in collaboration with the core developers of OpenFOAM from CFD-Direct Limited. With these developments, any user can execute an engine simulation with moving valves and piston over unlimited cycles. The functionalities and performance of AATE is demonstrated on a publicly available, non-proprietary engine case, TCC-III from University of Michigan. To make the benchmark case useful for the engine community, we demonstrate an automated meshing solution and provide examples of efficient reactive simulation setup and post-processing in engine context. The core engine solver will be available in future OpenFOAM-dev releases, while the TCC-III case will be available online separately.

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Shared Memory based Hybrid In-Situ Adaptive Tabulation of Vapor-Liquid Equilibrium Solutions and Detailed Chemistry

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Vapor-Liquid Equilibrium (VLE) model, a family of first-principled thermodynamic models for transcritical multiphase flows, faces computational challenges in multi-component systems. To address this, a novel ISAT-VLE method is developed, leveraging the in-situ adaptive tabulation (ISAT) technique to enhance computational efficiency and reduce memory usage by the tabulation. However, parallelizing ISAT-based CFD simulations encounters performance degradation as the number of cores increases due to the local to core nature of the ISAT table. To overcome this, a novel shared memory ISAT formulation using MPI-3 for CFD simulations is introduced, along with a hybrid ISAT retrieval algorithm incorporating both local and shared ISAT tables for optimal computational performance, efficient memory management, and predictive accuracy. A load-balancing algorithm within the shared memory architecture is also introduced to improve the parallel scaling of the ISAT model. Rigorous testing in high-pressure transcritical two-phase simulations demonstrates a significant speed-up factor (10 to 60) and controlled ISAT errors within 1%, showcasing commendable accuracy. The model is also extended to combustion simulations, integrating a shared ISAT-based tabulated dynamic chemistry model (TDAC), introducing an advanced and versatile approach for enhancing computational efficiency and accuracy.

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Development of high-order solver for ML-accelerated reacting flow simulations

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Recent advances in high-performance computing and artificial intelligence have enabled opportunities for the advancement of combustion engineering. One such possibility is the integration of machine learning (ML) with high-fidelity reacting-flow simulations for reliable predictions. However, ML for combustion is still limited by slow data transfer speeds between the CPU and GPU and legacy software. Therefore, we propose a new Discontinuous Galerkin (DG) solver built using the JAX library for high-performance simulations on CPUs, GPUs, and TPUs. The current work has two main advantages: Firstly, most numerical schemes for simulation of combustion problems employ lower-order finite volume discretization techniques, which may not sufficiently capture small-scale flow structures and reacting zones. In contrast, the DG method offers high-order accuracy on unstructured meshes with good dispersion and dissipation properties, with a high arithmetic intensity and lower memory requirements. Secondly, the use of JAX, a framework designed for ML applications, allows for a direct coupling

between the flow simulation and any ML applications. The resulting simulation framework will be demonstrated in application to online-learning of a transient flame configuration.

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Population-based optimization of complex reacting flows: Pilot study

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Optimization of complex reacting flows involving multi-component and multiphase flow phenomena is often challenging due to the unsteady and multi-scale nature of the flows. In this study, we present a computational strategy for model-free, population-based optimization of such flows. In the method, to optimize a set of flow parameters for targeted objectives, groups of simulation samples are distributed and iteratively search a parameter space until convergence. We evaluate the efficiency and accuracy of this method using canonical model problems. The method is implemented in an in-house compressible flow code to demonstrate optimization of three-dimensional high-speed reacting flows on multiple GPUs in a scalable fashion.

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Track18 Simulations with AI technologies

Track18-1 Simulations with AI technologies (1)

Chair: TBD
Wednesday, May 8; 10:40 - 12:20; Room K

Machine Learning Tabulation of Thermochemistry of Polycyclic Aromatic Hydrocarbon (PAHs) and Application to Turbulent Sooting Flames: An approach Combining DRGEP and HFRD-MMLP

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This work applies a machine learning tabulation methodology for the thermochemistry of combustion containing polycyclic aromatic hydrcarbons (PAHs), to accelerate the real-time computation of the large-size PAH mechanism in turbulent sooting combustion. This approach firstly uses DRGEP method to select a certain number of species from the PAH mechanism, and then proposes the hybrid flamelet/random data and multiple multilayer perceptrons (HFRD-MMLP) method to evaluate the concentration changes of selected species at every time step. The essence of the HFRD method lies in the generation of training data, which enhances the capacity of generalization for the reactive composition space encountered in practical turbulent combustion by using the random process to expand the training dataset from laminar flamelets. The MMLP artificial neural networks (ANNs) are then trained to predict different composition states, to improve the ANN prediction accuracy. To validate the effectiveness of the ANNs, they are initially tested on laminar flamelet simulations with varying strain rates and then on 1-D laminar premixed flames with varying equivalence ratio. Subsequently, tests are conducted on the Santoro laminar diffusion sooting flame and the DLR turbulent lifted sooting flame. The results regarding species mole fractions, temperature, PAHs and soot volume fraction show overall excellent agreement with the direct integration method. The proposed DRGEP-HFRD-MMLP method achieves speed-up factors of over 52 for the reaction step, in the LES-PDF simulation with the PAH mechanism in this work, surpassing the speed-up factors of approximately 12–14 and 16.2 in previous works on the GRI-1.2 mechanism for CH4/H2 combustion, and the DME mechanism, respectively. This indicates that the proposed machine learing method is highly effective for large size mechanisms in reducing the computational cost by replacing a significant number of highly stiff ordinary differential equations (ODEs) integration.

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Mitigating chemical stiffness in turbulent reacting flow simulations via an adaptive reduced-order model with time-dependent bases

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Direct Numerical Simulation (DNS) of turbulent reacting flows is often prohibitively expensive for practical engineering problems due to the large number of transport equations involved and the wide range of length and time scales associated with turbulence and combustion. Reduced-order models (ROMs) can dramatically reduce the number of transport equations, mitigating the cost of high-fidelity simulations with a minimal sacrifice in accuracy. However, identifying low-dimensional representations of the high-dimensional thermochemical state often depends on offline training, restricting such ROMS to conditions similar to that of expensive, pre-existing high-fidelity training datasets. Recently, a novel ROM approach named time-dependent bases with CUR decomposition (TDB-CUR) was proposed that adaptively constructs and updates a ROM in time by leveraging physics and the instantaneous thermochemical information instead of expensive training data. Though promising, the initial formulation of TDB-CUR does not directly reduce the computational cost associated with stringent time step requirements imposed by stiff chemical systems. The present work aims to further reduce the computational cost of TDB-CUR by increasing the allowable time step. Present improvements are benchmarked against canonical turbulent reacting flows, demonstrating as much as an order of magnitude reduction in computational cost as compared to the original TDB-CUR formulation.

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Optimizing Mesoscale Combustor Power using Taguchi Orthogonal Array, Computational Fluid Dynamics and Machine Learning

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With technological advancement, there is an increasing shift towards miniaturizing engineering systems . Ensuring electric power to these miniature systems using compact power sources is a concern. Compared to batteries, mesoscale combustors offer better energy density and can provide instantaneous power through combustion. Designing a compact combustor with maximum power output plays a critical role in developing this kind of power system. Stepped combustors are suited for better flame stability under varying power output . The different geometric parameters of the step combustor, such as step length and step diameter, impact the combustor's performance and power output. Designing a stepped combustor with optimum geometric parameters to achieve maximum power output is tedious using conventional numerical or experimental methodologies. Machine learning (ML) techniques can be utilized to arrive at an optimal design with fewer design iterations. This work optimizes the combustor geometry to achieve maximum radiation power from the combustor walls for a Thermophotovoltaic (TPV) system. The proposed methodology utilizes the Taguchi method, Computational Fluid Dynamics (CFD), and neural networks. The number of CFD simulations used to train the neural network is reduced using the Taguchi orthogonal array method. Next, the premixed H2/air combustion simulations are carried out for the design space obtained from Taguchi method. Finally, using the simulation data, a Back Propagation Neural Network (BPNN) technique is used to achieve the optimal step diameters . The method significantly reduces the design space and time to obtain the configuration with maximum radiative power.

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React-DeepONet: A Combustion Chemistry Acceleration Framework for CFD

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A combustion chemistry acceleration scheme for implementation in reacting flow simulations is developed based on deep operator nets (DeepONets). The scheme is based on a mapping of a subset of the thermochemical scalars' vector between incremental and adaptive time steps. The subset corresponds to variables that are adequate to represent the evolution of the chemical system. The DeepONet-based scheme also relies on a mapping of the solution of this subset onto a corresponding solution at an adaptive time increment to overcome the restrictive requirements of integrating such solutions with stiff chemistry. Training for the DeepONet is also implemented differently from previous approaches to the solution of PDEs with DeepONets. Instead of constructing solutions from their initial to their final states using DeepONets, the training relies on prescribed short-horizon time windows for training where intermediate solutions also serve as initial states for training. An additional framework of latent-space kinetics identification with modified DeepONet is proposed, which enhances the computational efficiency and widens the applicability of the proposed scheme. The scheme is demonstrated on the "simple" chemical kinetics of hydrogen oxidation and the more complex chemical kinetics of n-dodecane high- and low-temperatures. The proposed framework accurately learns the chemical kinetics and efficiently reproduces species and temperature temporal profiles. Moreover, a very large speed-up with a good extrapolation capability is also observed with the proposed scheme. Measures of enforcing element/mass conservation as well as integration of the framework within a CFD code are implemented showing important speed up and memory saving with a CFD simulation.

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Track18-2 Simulations with AI technologies (2)

Chair: Michael E Mueller
Co-Chair: Hiroshi Gotoda
Wednesday, May 8; 13:30 - 15:10; Room K

Surrogate modeling of the methane diffusion combustion field using the pseudo-time stepping-based physics-informed neural networks

Zhen Cao, Kun Luo, Kai Liu, Yuzhou Cheng, Liang Jiang, Zhentao Pang, Jianren Fan
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The physics-informed neural networks (PINNs) has emerged as a popular deep learning framework extensively applied in the field of computational science, particularly in computational fluid dynamics (CFD). In this study, we propose a novel PINNs framework based on the concept of pseudo-time stepping (PTS-PINNs), inspired by the traditional approach in CFD. The proposed framework

is validated through experimental investigations of the two-dimensional steady-state methane laminar diffusion combustion. The results demonstrate that the conventional PINNs framework encounters difficulties in training the methane combustion process and requires the initialization of a high-temperature field to ensure the correct convergence path. In contrast, the pseudo-time stepping-based PINNs exhibits the ability to rapidly converge from a random initial field to the final stable combustion state, with a relative error of less than 10% compared to the traditional CFD numerical solution. The effectiveness of PTS-PINNs in solving the combustion system can be attributed to its convergence path aligning with the physical evolution direction. In contrast, traditional PINNs tend to converge towards the direction of minimizing the loss function, which may not necessarily align with the laws of physics. In summary, the PTS-PINNs framework presents a promising avenue for neural network solutions in combustion systems.

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Prediction of laminar burning velocity for premixed ternary ammonia/hydrogen/methane-air flames using ensemble learning

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Zero-carbon fuels, such as hydrogen and ammonia, play a crucial role in the energy transition by providing cleaner alternatives to natural gas (methane), particularly in industrial combustion systems. Binary and ternary blends of these fuels offer a transitional, low-carbon solution in the near future. Laminar burning velocity (LBV), a fundamental combustion property, varies significantly for ammonia, hydrogen, and methane. While the LBV of binary blends of these fuels has been extensively studied, research on ternary blends is limited. This study aims to utilise ensemble learning approach to predict the LBV of ternary ammonia/hydrogen/methane-air mixtures for a large parameter range. The training dataset comprises experimental data from numerous publications (>90 papers) and synthetic data generated through 1D freely propagating premixed flame simulations in Cantera, using a detailed chemical kinetic mechanism. Three machine learning (ML) algorithms –artificial neural networks (ANN), Gaussian process regression (GPR), and extreme gradient boosting trees (XGBoost)– are trained, validated and optimised. Subsequently, a simple ensemble averaging method is employed to mitigate overfitting and enhance robustness. The ensemble model achieves a R2 of 0.991, with an inference time approximately 8,000 times faster than the 1D simulation run time. The final ensemble model offers efficient and accurate predictions LBVs for ammonia/hydrogen/methane-air mixtures at T = [295–756K], P = [1–10bar], φ = [0.5–1.8] and all possible blending ratios, enabling discovery of conditions that have not been studied experimentally.

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Three-dimensional Convolutional Neural Networks for Enhanced Turbulence Modeling in Large-eddy Simulations of Partially Premixed Swirl Flames

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Three-dimensional convolutional neural networks for enhanced turbulence modeling in large-eddy simulations of partially premixed swirl flames subgrid-scale (SGS) phenomena in reacting flows, such as partially premixed swirl flames. These flows exhibits challenges like pressure expansion, abrupt density reduction, and stiff viscosity increase, which are not adequately captured by standard eddy-viscosity models or conventional data-driven approaches like fully connected neural networks (FCN). This study introduces an advanced three-dimensional convolutional neural network (3D-CNN) designed to accurately model SGS stresses and scalar fluxes. This model, leveraging spatial inputs of first-order velocity and scalar gradients across local and adjacent grid points, effectively captures the SGS dynamics of turbulent combustion without relying on eddy-viscosity assumptions. In a-priori tests comparing the proposed 3D-CNN with traditional models such as the Smagorinsky model (SM), velocity gradient model (VGM), and FCN, the 3D-CNN demonstrates superior performance in predicting SGS variables, evidenced by higher correlation coefficients. Additional posteriori tests confirm the model's applicability and effectiveness in LES codes. This research underscores the value of integrating spatial inputs and 3D convolutional networks in enhancing the accuracy and generalizability of SGS turbulence models for turbulent combustion LES.

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Deep learning for sub-filter density function prediction in turbulent combustion

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Presumed filtered density function (FDF) approaches are widely used in sub-grid scale (SGS) modelling for turbulent combustion simulation. However, this numerical approach brings challenges for several conditions of interest, such as combustion with extinction and reignition and multi-regime burners. Many recent studies have demonstrated that the artificial neural network (ANN) is a suitable candidate. On the other hand, the FDF prediction highly depends on the training dataset due to the ANN's limitations in extrapolation, which limits the application of the ANN in practice.

Concurrently, generative models have exhibited improved predictive ability in language and vision with high generality and have been leveraged in biology and materials engineering. This work develops a diffusion model to generate the joint FDF of the progress variable and mixture fraction by inputting the first and second moments of these two key variables. Through the training with limited data of MILD (Moderate, Intense and Low Dilution) combustion, this model illustrates an improved performance than the conventional ANN for a variety of conditions, including MILD combustion at different dilution levels (not used in the training sets), various filter sizes and other flame cases. The detailed results and analysis will be discussed during the presentation.

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Simulation of supercritical CH4/O2 flame with hybrid data-physics based machine learning method

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We developed a highly accurate thermodynamic property and reaction source term surrogate model using a hybrid canonical and random data sampling method. The thermodynamic network is an MLP model with three hidden layers and ODE network is a multi-segment network. Depending on Chemical Explosion Mode Analysis (CEMA) theory, the first stage identified the combustion modes (explosive mode, decaying mode, etc.). The explosive mode needs to enter the second stage which is used to predict reaction source terms. And the remaining modes are assumed to be inert and skip the chemical computation. These models are applied to supercritical CH4/O2 flame with Homogeneous Isotropic Turbulence (HIT). A neural network with 40,000 neurons and 5.6 million training data achieves good agreement in major thermodynamic properties such as density, viscosity etc. For the ODE surrogate model, we found that the average reaction rate in the inert region does not change significantly, which are redundant noise points for the chemical network. Filtering out inert zone data reduces the MAE and training epochs of networks with the same parameter by 50% and the predictions for major and minor components exhibit good consistency. The average computation time for thermodynamic property and reaction source terms is reduced by a factor of 10, and memory consumption is only within 20MB.

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Track18-3 Simulations with AI technologies (3)

Chair: Hiroshi Gotoda
Thursday, May 9; 09:50 - 12:30; Room F

Hybrid LES-CFD modeling with machined learning methodology on Tangentially-Fired Coal Combustion System

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High-fidelity modeling is a valuable tool for investigating complex multi-scale multi-physics mechanisms in industrial-scale coal combustion. However, deploying these models for industrial applications requires additional steps to enhance accuracy. This work introduces a hybrid LES-CFD model with a machine learning approach to improve predictive capabilities by quantifying uncertainty from prediction results and experimental data. The analysis builds on high-fidelity LES-CFD simulations for industrial-scale coal combustion. The newly proposed machine-learning model integrates Bayesian-based and Bound-to-Bound models, defining predictivity through statistical inference from information propagated from models and experiments.

This research successfully applies the hybrid methodology to coal combustion in a GE-Alstom's pilot-scale BSF. The outcomes advance model prediction accuracy for key quantities of interest (QoI's): heat flux to the wall, gas temperature, and oxygen concentration. Machine learning

expands the parameter space, ultimately finding consistency between simulation and experiment. Predictions are bound with quantified uncertainty, providing informative insights for industrial applications. The analysis informs modelers and experimentalists of allowable ranges for simulation input parameters, ensuring useful predictions.

The predictivity produced by this method directly informs the optimization of industrial combustion system operations, bridging high-fidelity modeling with lab results to real engineering applications. Moreover, this research exemplifies the power of the hybrid approach, combining high-fidelity simulation with machine learning methodology, applicable to a wide range of complex emerging problems.

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Detailed simulation of LOX/GCH4 flame-vortex interaction in supercritical Taylor-Green flows with machine learning

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This study introduces detailed computational analyses of liquid oxygen and methane (LOX/GCH4) combustion in a Taylor-Green vortex (TGV) configuration, under supercritical conditions–significant for the development of rocket engines, industrial powertrains, and modern gas turbines. We adapt the classical three-dimensional TGV test case, incorporating real fluid behaviour, to explore the dynamics of reactive flows at extreme pressures and temperatures. The simulation contrasts the conventional ideal gas approximation with the Peng-Robinson (PR) cubic state equation, highlighting the pronounced effects of substantial density variations inherent in real gases on flame behaviour and vortex dynamics. Enhanced flame stretching and quenching are observed with real fluids, as opposed to their ideal counterparts. To mitigate the high computational demands of calculating real-gas thermophysical properties, we employ a deep learning framework with deep neural networks (DNNs). This novel approach is validated against the reactive TGV configuration, showing high predictive fidelity and a 13-time increase in computational efficiency compared to traditional methods. This research not only sets a reference point for subsequent investigations into three-dimensional supercritical flame-vortex interaction but also suggests that leveraging machine learning could substantially advance the high-fidelity simulation of supercritical combustion.

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Reducing memory requirements of In-Situ Adaptive Manifolds using neural network coupled binary trees

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Manifold-based combustion models can decrease the cost of turbulent combustion simulations by projecting the thermochemical state onto a lower-dimensional manifold, allowing the thermochemical state to be computed separately from the flow solver. Solutions for the manifold equations have been traditionally precomputed and pretabulated, resulting in large memory requirements and significant precomputation cost even for simple problems. In-Situ Adaptive Manifolds (ISAM) allows for solutions to the manifold equations to be computed as the simulation progresses and stored using binary trees with In-Situ Adaptive Tabulation (ISAT), allowing for the use of more general models. While ISAT has helped reduce the memory requirements from previous pretabulation approaches, as the model complexity grows, the memory requirements of ISAT will eventually become too large. In this work, neural networks are used to replace portions of the binary tree within ISAT to decrease the memory requirements of the ISAT database. Analysis of the trade-off between fewer, larger, more global neural networks each replacing more leaves and more, smaller, more local neural networks each replacing fewer leaves is explored in detail including both memory and retrieval time. Data from a Large Eddy Simulation of a canonical turbulent flame is used to analyze this trade-off.

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High-resolution three-dimensional reconstruction of velocity for turbulent flames with physics-informed neural networks

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In the field of combustion diagnostics, the simultaneous measurement of velocity and temperature in three dimensions is desirable for gaining fundamental insights into the turbulent flames and developing numerical predictive tools. However, such measurements often face challenges due to the high cost of optical devices, complex calibration procedures, and data acquisition. In the present work, for the first time, a novel physics-informed neural networks (PINNs) framework is established to alleviate the measurement challenges. This framework enables three-dimensional high-resolution reconstruction of turbulent combustion for velocity, based on two-dimen-

sional velocity planes and available three-dimensional temperature fields. The performance of the PINNs is evaluated on two different configurations of turbulent flames without and with a mean shear, including freely propagating planar premixed combustion and swirling combustion. The reconstructed fields of velocity are compared with the high-fidelity direct numerical simulation (DNS) data, and both qualitative and quantitative analyses are performed for the model performance evaluation. This study highlights the potential of PINNs as a complement for combustion diagnostics and provide new insights for the development of physics-informed machine learning methods in combustion research.

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Multi-Component Temporal Clustering Analysis in Reaction Phase Space for Hydrogen Jet Flames

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Worldwide push towards clean energy requires new technological pathway and energy carriers. Hydrogen is an ideal candidate given its high calorific value and reduced emissions; however, the operational risks are heightened due to phenomenon like flashback. Detailed numerical investigations have revealed complex interaction between strain effects, caused due to varying flow structures, and flame reaction zones affecting flame stabilization. A data-driven approach to classify different flame branches in reaction phase space for strained hydrogen jet flames is implemented, and identification of ignition-extinction cyclic pathways on this classification is demonstrated. The dataset is generated from a reactive jet-in-crossflow simulation, with experimental validation. Each temporal snapshot contains multiple fields like OH, progress variable, reaction source term etc. Clustering procedure is applied to the time-evolving dataset and the resulting time-axis modes are embedded with dynamically similar field variations defined over the selected time interval. Spatially, the modes are discrete and non-overlapping, and a unique dynamical pattern can be isolated. This presents a clear interpretation of dominant spatial length-scales and correlations as a function of the isolated dynamical pattern represented by the corresponding phase space centroid. The approach improves understanding of localized source terms under varying strain effects and the associated flame dynamics.

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Unveiling Flame Characteristics for Combustion Process of Ammonia Blends using Machine Learning

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Direct combustion of ammonia is being actively considered as a carbon neutral fuel. However, due to its low laminar flame speed and propensity to produce high NOx emissions, it is generally blended with natural gas and hydrogen to improve its combustion characteristics. Developing a viable combustor using physics-based models like Computational Fluid Dynamics (CFD) is computationally expensive and finding its optimal operating parameters using such tools is difficult. Therefore, this paper demonstrates the efficacy of replicating important CFD results from a surrogate model built using Artificial Neural Network (ANN) based Machine Learning tools. This CFD model was based on a semi-detailed NH3/H2/CH4/n-C12H26 mechanism consisting of 242 species and 1769 reactions including both nitrogen oxides (NOx) and soot sub-mechanisms. CFD simulations were performed in the parameter space of blend ratios, operating pressures and mass flux ratios of a jet flame at limited discrete points following a SOBOL sequence and flame responses are estimated. ANN is utilized to build a surrogate model among the aforementioned parameters and response variables, which in turn can predict the frame characteristics for several other unknown operating conditions. This quasi-random low-discrepancy SOBOL sequence not only helps represent the parameter space uniformly and thereby requires a minimum number of CFD simulations to identify the space but also preserves sampling points where simulations have been already performed while creating new sample points.

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Machine learning implemented large eddy simulation of turbulent premixed flames by an AI-assisted fractal dynamic sub-grid scale (FDSGS) model

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Large eddy simulation (LES) of turbulent premixed flames which is implemented with machine learning has been realized with an AI-assisted sub-grid scale (SGS) combustion model. The AI-assisted SGS combustion model adopted in this research is developed based on the fractal dynamic SGS (FDSGS) model which was developed

in our previous research. In the FDSGS model, a model parameter related to local Kolmogorov length scale is included. In the present study, by using fully connected neural network or fully convolutional network (FCN), it was shown that local Kolmogorov scale is estimated with higher accuracy by the machine learning and the prediction of SGS burning velocity is improved through static tests. The static tests are conducted using direct numerical simulation (DNS) data of freely propagating turbulent premixed flames, turbulent jet premixed flames and turbulent V-shape flames. This AI-assisted FDSGS model is then implemented on our LES code, realizing the possibility of local Kolmogorov scale estimation with different combustion configurations such as flame shapes or filter widths. A dynamic test of the AI-assisted FDSGS model is conducted by LES with machine learning implementation for turbulent jet premixed flame. It was shown that the prediction of flame surface area and average temperature distribution by the AI-assisted model is more accurate than that by conventional SGS combustion models including the non-AI-assisted FDSGS model.

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Track18-4 Simulations with AI technologies (4)

Chair: TBD
Friday, May 10; 09:50 - 11:50; Room D

Kinetic reduction for efficient turbulent combustion kinetic uncertainty quantification via active subspace enabled by neural network

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Propagating uncertainties in kinetic models through combustion simulations provides important reliability and accuracy metrics, but remains challenging and costly especially for large kinetic models and expensive turbulent simulations. Surrogate model and dimension reduction techniques were previously applied to facilitate such analysis, but these are often limited to low-dimensional, simple cases with scalar solution targets. Here, we developed a neural network-accelerated framework for identifying a low-dimensional active kinetic subspace that can capture the mixture fraction and strain rate effects of kinetic uncertainty across the entire temperature solution space of a flamelet table. We demonstrated the computational savings enabled by this framework with a flamelet-based application in a Reynolds-averaged Sandia Flame D simulation using a 217 reaction model. By leveraging the large dimensional compression efficiency of the active subspace method, offloading the gradient sampling onto the laminar flamelet simulations, and accelerating computation via a specifically designed neural network, we estimated the uncertain temperature profiles in this turbulent flame with strong 70-85% accuracy using just seven perturbed solutions. The subspace is identified within the flamelet table and does not scale in cost with the complexity of the combustion model, indicating promise for future application to larger-scale and more complex turbulent combustion applications.

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Jacobian-Informed Clustering for Sample-Partitioning Adaptive Reduced Chemistry Methods

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Unsupervised learning methods are gaining prominence in the combustion modeling community for their ability to identify important data patterns, enhancing the efficiency of Reduced Order Models. Traditionally, clustering algorithms rely on the minimization of statistical measures like Euclidean distance or Local PCA-based reconstruction error (VQPCA), potentially leading to suboptimal solutions for combustion applications.

This study emphasizes the importance of guiding the solution toward more physics-grounded clusters in the context of Adaptive Chemistry Simulations, where identifying locally homogeneous zones is crucial for the model's performance. For this aim, we adopt the Jacobian Scaled K-means clustering formulation (JSK-means) within the eSPARC methodology framework. This clustering algorithm seeks to minimize an objective function modified by scaling matrix cast as the chemical Jacobian at the cluster's centroid. Such matrix, acting as a linear transformation on the distance vector, ensures that two points, that are near in the composition space, share similar dynamical characteristics (i.e., similar chemical source terms).

Results show that JSK-means allocates more clusters in the active thermochemical regions, with respect to VQPCA, to better highlight the source term variations. As a consequence, the chemistry reduction generates a library of more compact local mechanisms resulting in a smaller average number of species to be solved in CFD.

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Deep learning-based chemical kinetic surrogate model with strictly enforced conservation laws

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In combustion simulations, the stochastic nature of artificial neural network (ANN) presents a notable obstacle in upholding physical principles, casting a shadow over the reliability of data-driven methods. To address this limitation, we introduce a novel approach called the Physics-Constrained Neural Network (PCNN) as surrogate models for chemical source terms. This method strictly enforces predictions to preserve conservation laws, including mass, energy, and element conservation. The performance of PCNN with both the original ANN and the popular physics-informed neural network (PINN) are compared across various combustion scenarios, including zero-dimensional autoignition, one-dimensional premixed laminar flame, two-dimensional triple flame, and outwardly expanding turbulent spherical flame. Our results reveal that small errors of ANN predictions can lead to severe violations of physical principles because ANN's statistical description does not contain physical information. Such error accumulation in continuous evolutions accounts for ANN's non-physical predictions. In contrast, PINN and PCNN exhibit superior robustness compared to ANN by incorporating conservation laws. Particularly, PCNN demonstrates effectiveness in providing stable and accurate predictions by suppressing error accumulation, while maintaining high computational efficiency. Our study underscores the critical role of fundamental physical principles in the development and applications of machine learning based methods.

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Large eddy simulation of swirling flames: GPU/DNN-accelerated finite rate chemistry

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Swirling flow, renowned for its ability to stabilize lean premixed turbulent flames, has found extensive application in gas turbines to meet increasingly stringent low-emission constraints. Numerous numerical simulations, employing various combustion models and mesh resolutions, have been undertaken on laboratory-scale flames to gain deeper insights into swirling flame dynamics. Despite these efforts, a persistent challenge remains: striking a balance between achieving high-fidelity results and maintaining low computational costs, especially in cases where combustion models involve direct solving of finite-rate chemistry. This study addresses this challenge by integrating a deep neural network (DNN) into a GPU-based solver. The focus is primarily on assessing the effectiveness of the proposed GPU/DNN approach through two large eddy simulations of swirling flames. The simulation outcomes reveal a commendable agreement in flow and flame structures between the GPU/DNN approach and the conventional CPU-based solver with direct integration (DI). This comparison suggests that the GPU/DNN approach can attain the same level of accuracy as the conventional CPU/DI solver. Furthermore, the overall speed-up factor achieved by the GPU/DNN approach exceeds two orders of magnitude. This investigation establishes a potential foundation for fully resolved laboratory-scale flame simulations based on detailed chemistry, offering a considerably more cost-effective computational solution.

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