IP1

Modeling Flame Holes in Turbulent Nonpremixed Flows

Turbulent diffusion flames can be quenched in regions of high strain owing to increased heat loss away from the reaction zone. These chemically inert regions are sometimes called flame holes (Dold et al. 1991). Turbulent flames with extinction are relevant in modern combustors where the flame temperature is kept low to reduce pollutant formation or in lifted jet flames used for thermal protection of the burner. Modeling the dynamical behavior of flame holes, without recourse to a detailed chemical-transport description, requires new numerical methods that describe the evolution in time of the flame boundary (or rim) on the moving stoichiometric surface. The kinematics of the flame rim is normally approximated as those of a two-dimensional edge flame whose speed of propagation is controlled by the local strain. In mathematical terms, the challenge is the efficient numerical evolution of a state field defined on a two-manifold (of varying shape, and possibly multiply connected). In this talk, I will describe recent progress on the numerical and physical modeling of flame holes as it applies to turbulent nonpremixed flames. Special emphasis of current research is to achieve high-order of accuracy, flexibility, and robustness, while maintaining relatively low computational cost.

Carlos Pantano
Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
cpantano@illinois.edu

IP2

Progress and Challenges in Simulating Combustion Systems with Realistic Chemistry

The vital role of simulations and computational insights in reducing pollutant emissions, designing better engines and better fuels, and assessing the technical and economic viability of radically different combustion technologies, is now clearly established. A key enabling step is the development of computational approaches that allow our increasingly detailed knowledge of the chemical kinetics of realistic fuel oxidation to be applied to the modeling and simulation of combustion reactors. In this talk, I will briefly review the challenges associated with the integration of detailed chemical kinetics in reactive flow simulations. I will then discuss the progress we have made in the analysis and reduction of complex kinetic networks, with a focus on graph-based techniques and the characteristics of the stand-alone reduced models they typically generate. Using Large-Eddy Simulations of turbulent flames as case study, I will show how these techniques are enhanced through careful integration and coupling with CFD tools, wherein the flow characteristics adaptively inform the reduced chemical model to be used. I will conclude on the remaining challenges still to overcome, and potential avenues to do so.

Perrine Pepiot
Cornell University
pp427@cornell.edu

IP3

Dynamic Partitioning and Quantum Speedup for Turbulent Combustion Simulation

Within the past thirty years, a variety of subgrid scale closures have been developed for large eddy simulation (LES) of turbulent combustion. The filtered density function (FDF) is one of such closures and has proven very effective in a variety of applications. Despite its demonstrated capabilities, the computational cost associated with FDF can be expensive compared to other (more conventional) methods. This problem can be effectively alleviated by taking advantages of modern developments in computing and information science. A novel strategy is to couple an architecture aware graph partitioning algorithm with a dynamic (re)partitioning framework. This provides an optimal load balance, while minimizing the cost of data migration. Each of the partitions is treated via an entirely self-contained solver (in either Eulerian or Lagrangian contexts). The communication between the solvers is local, and shared information is limited to neighboring partitions. Quantum computing is also very promising for future LES via FDF. Recent developments in quantum enhanced measurements provide an algorithm that facilitates a quadratic speedup over classical FDF solvers. This demonstration identifies FDF as a viable problem to take advantage of speedups offered by future quantum computers.

Peyman Givi
University of Pittsburgh, USA
Givi@engr.pitt.edu

CP1

High Explosive Performance Modeling Using the Pseudo-Reaction Zone Energy Release Model in Programmed Burn

Programmed Burn (PB) methods were developed to calculate timing and detonation energy delivery in high explosive (HE) engineering systems without resolving the reaction zone length and time scales. These methods precompute the detonation wave motion, triggering energy release only upon the wave's arrival. Given the primary aim of accurately describing the energy delivery to surrounding materials, the PB methodology avoids resolving the detonation reaction zone required in reactive burn. Advanced PB methods use a surface evolution model known as Detonation Shock Dynamics (DSD) to provide time-of-arrival and front shape information throughout the geometry of interest. As the timing and energy release components are weakly coupled, the success of the PB method relies on the energy release rate being optimally synced to the DSD surface wave motion. We will detail a calibration methodology of the Pseudo-Reaction Zone (PRZ) energy release model that achieves this aim, and apply it to the plastic-bonded HEs PBX 9501 and 9502. The PRZ model is defined by a two-step reaction rate dependent on the surface normal detonation velocity provided by DSD (Wescott, 2007). The calibration procedure compares multi-dimensional simulations of detonations in 2D axisymmetric rate-sticks and planar slab geometries based on the PRZ rate law to the equivalent DSD-generated steady-state front shapes and phase velocities. We also discuss strengths and limitations of the DSD/PRZ energy delivery model.

Carlos Chiquete, Mark Short, Chad Meyer, James Quirk
Los Alamos National Laboratory
chiquete@lanl.gov, short1@lanl.gov, chadmeyer@lanl.gov, quirk@lanl.gov

CP1

Mesoscale Simulations of Energetic Materials Using Density-Based Kinetics

In this work we present results for the initiation of det-

onations in energetic materials through power deposition due to pore collapse. We solve the reactive Euler equations, with the energy equation augmented by a power deposition term. The deposition term is based on previous results of pore collapse at the microscale, modelled at the macroscale as hot-spots. We assume a one-step kinetic model. Previous results used Arrhenius kinetics; however, late time solutions developed instabilities, a well-known problem when using temperature-based kinetics. Therefore in this work we replace the Arrhenius kinetics with one based on density. Simulation results show that a critical size of the hot-spots exists. If the hot-spots exceed the critical size, direct initiation of detonation results. We also carry out two-dimensional simulations, where the microstructure is generated by a random packing code, developed specifically for packing energetic crystals. The crystals are then seeding by randomly placing hot-spots based on varying void content. Go-no go results as a function of shock pressure are presented.

Thomas Jackson
University of Florida
tlj@ufl.edu

Ju Zhang
Florida Institute of Technology
jzhang@fit.edu

CP1

Numerical Simulation of Detonation Propagation in Practical Geometries

Rotating detonation engines (RDEs) are re-emerging as one approach to increasing efficiency of conventional gas turbines. The pressure gain associated with such devices can be used to derive extra work. The development of robust RDEs depend on the design of fuel injectors that can withstand detonation conditions while preventing backflow of combustion products into the feedline. In this regard, the availability of numerical simulation tools that can capture detonation wave propagation through incompletely mixed fuel and air will directly benefit RDE development. Here, a high fidelity finite volume LES based Navier-Stokes solver is formulated for detonation applications on unstructured grids, using the OpenFOAM framework. A detailed chemistry representation is used to describe detonations. The method is applied to complex flow geometries that replicate the main features of the injection region in a practical RDE. Results obtained using this computational tool will be compared to DNS data from an in-house code for detonation based flows on structured grids, for validation purposes and model optimization. Numerical and modeling issues related to such configurations will be discussed.

Damien Masselot, Takuma Sato, Venkat Raman
University of Michigan
masselod@umich.edu, takusato@umich.edu, ramanvr@umich.edu

CP1

Condensed-Phase Oblique Detonation Interaction with a Rigid Wall

We examine the wave reflection patterns generated by the interaction of a detonation in a condensed phase explosive impacting obliquely onto a rigid wall. The computational approach uses a shock-fit methodology (A. Henrick, Ph.D. Thesis, Univ. Notre Dame, 2008; Aslam and Romick, 15th Detonation Symp., 2014) with a second-order finite volume algorithm. We look at the reflection patterns created by an instantaneous reaction Chapman-Jouguet detonation, compared with those of a small, resolved heat release detonation (Bdzil, J. Fluid Mech., 1981), where the first part of the reaction is instantaneous, but the second has a finite length scale. We compare the results of the computations with an asymptotic study recently conducted by Bdzil and Short (J. Fluid Mech., 2016, to appear) for small oblique detonation incident angles.

Mark Short
Los Alamos National Laboratory
short1@lanl.gov

John Bdzil
University of Illinois at Urbana-Champaign
jbbdzil@gmail.com

Carlos Chiquete, Chad Meyer
Los Alamos National Laboratory
chiquete@lanl.gov, chadmeyer@lanl.gov

CP1

Modeling of Aluminum Combustion in An Oxidizing Environment with the Gibbs Formulation

We present a model for aluminum combustion in an oxidizing enviroment that employs the newly-developed Gibbs formulation, which presumes a single local equilibrium stress tensor and temperature at each point in the material. This multi-component formulation considers solid and liquid phases of aluminum and its oxide and the gas phase of aluminum, oxygen, and nitrogen. Phase changes and exothermic reactions are characterized as reactions or phase change. The order parameters that are often invoked in similar models are simply the mass fractions of the component species. Each change process has its individual reaction rate. The Maxwell-Stefan model is used for diffusion. In oxidizing environment, pre-heated meso-scale aluminum slab partially coated with its oxide is heated, and different ignition transients are observed when the oxide concentration in the layer iv varied; the more aluminum oxide concentration in the layer, the lower the magnitude of the observed thermal spike near the layer during ignition.

D. Scott Stewart
University of Illinois
Dept of Theor & Applied Mech
dss@illinois.edu

CP1

A DSD Model for Converging Detonations

We derive the detonation shock dynamics (DSD) regularity-condition with a simple expansion of the Hugoniot equation for a general equation of state. We explicitly integrate the regularity-condition for a JWL equation of state with a quadratic expansion about the sonic specific volume around the ZND state for a converging detonation with a symmetrical geometry. We also numerically integrate the regularity-condition without approximation and obtained consistent results. The integral curves agree with the data from direct-numerical-simulations. In addition, we have calibrated a detonation front evolution-equation for a practical HE materiel. A particle-based DSD front tracker produces detonation front geometries closely matching the DNS data for both converging and diverging waves using this evolution equation. Thus, we conclude that the detonation-shock-dynamics can be used for mod-

elling a converging detonation as well as for a diverging detonation.

Jin Yao, Laurence E. Fried, Peter A. Vitello
Lawrence Livermore National Laboratory
yao2@llnl.gov, fried1@llnl.gov, vitello@llnl.gov

CP2

A Computational Study of Ionic Wind Effects on Dynamics of Nonpremixed Counterflow Flames Subjected to DC Electric Fields

Previous experimental studies reported significant effects of the imposed electric field on the dynamics and structure of the flames. However, the role of the ionic wind generated by the applied electric field needs further investigation in order to provide fundamental understanding of the complex interactions of the electric fields and the flame-generated ions and electrons. In this study, high fidelity simulations were performed to describe the effects of DC electric fields on the behavior of nonpremixed counterflow flames with an emphasis on the modification of the velocity field caused by the ionic wind. The distribution of the charged species, electric field and current is computed based on detailed two-dimensional numerical simulations using approaches similar to previous studies. The ability of the model to predict the flame behavior is assessed by comparing to available experimental measurements. Results show that the presence of the electric field affects the strain rate and the location of the reaction zone. The movement of positive and negative ions in opposite directions towards the cathode and anode, respectively, generates a bidirectional ionic wind, which decreases the flow local velocity. As the majority of ions are positive, the flame is moved toward the cathode. An interpretation of the stabilization mechanism of the flame under a bias voltage is proposed based on an analysis of the current-voltage characteristics.

Memdouh Belhi
Clean Combustion Research Center, King Abdullah University
of Science and Technology (KAUST), Saudi Arabia
memdouh.belhi@kaust.edu.sa

Bok Jik Lee, Hong G. Im
King Abdullah University of Science and Technology
bokjik.lee@kaust.edu.sa, hong.im@kaust.edu.sa

CP2

Simulation of Plasma Initiation in Liquid Medium

In spite of the great deal of research emphasized on application of plasma in liquids, only a limited number of reported works have focused on the understanding of the underlying physics. In the current work, an attempt is made to present a mathematical model to describe the initial stage of plasma discharge formation in a liquid medium. The model is based on a density based compressible solver solving for the electrical field, momentum, energy and species conservation together with plasma reaction kinetics to resolve the inter coupled physic-chemical processes. Three different electric body forces including the ordinary electrostatic force, force acting on an inhomogeneous dielectric and force appearing due to electric field gradient are considered. The multiphase effects are also considered by including a multi-fluid flow model, surface tension model together with a special treatment of interfacial electric forces. The comprehensive model is able to provide insight on the role of different dielectrics, interface location and applied electric pulse profile.

Ali Charchi Aghdam, Tanvir Farouk
University of South Carolina
alic@email.sc.edu, farouk@cec.sc.edu

CP2

DNS of Partially Premixed Mild Combustion

DNSs of partially premixed MILD combustion have been performed in the present work by extending the methodology of Minamoto et al. (CST **186** 1075-1096 (2014)) to include spatial variation of the mixture fraction, Z. Three different cases were performed by varying in a first step the ratio of length scales between the initial progress variable, c, field and the Z field from $L_c/L_Z < 1$ to $L_c/L_Z \approx 1$ and in a second step by increasing the dilution level of oxidizer with flue gases. The initial turbulence field for all cases is kept the same and the chemical mechanism used is based on SMOOKE methane-air mechanism which is extended to include OH* chemistry. The inclusion of OH* chemistry will allow to finely distinguish regions of actual heat release in MILD combustion from OH in the recirculating exhaust gas. Preliminary results have shown that reactions zones present a complex morphology, extremely different from classical combustion with a deeply convoluted aspects and high interaction between reaction zones. Additional analysis highlighted that reactions were occurring mostly in lean mixture with the reaction zones seemingly wrapped around pockets of rich mixture. Furthermore, it was observed that decreasing the oxygen level leads to reactions occurring over larger regions in the physical domain. Future work will be devoted to further qualify the structure of the reaction zones and assess the suitability of OH* to indicate heat release in MILD combustion.

Nguyen Anh Khoa Doan, Nedunchezhian Swaminathan
University of Cambridge
nakd2@cam.ac.uk, ns341@cam.ac.uk

Yuki Minamoto
Tokyo Institute of Technology
yminamot@navier.mes.titech.ac.jp

CP2

A Spectral Deferred Correction Strategy for Low Mach Number Reacting Flows Subject to Electric Fields

We propose an algorithm for low Mach number reacting flows that includes the chemical production and electrical field forcing of charged species in the flame zone. The work is an extension of a multi-implicit spectral deferred correction (MISDC) algorithm that is designed to advance the solution in time at scales associated with the advective transport, and is applicable to cases where local separations in net charge give rise to dielectric relaxations and nontrivial interactions with externally applied electric field. In the scheme diffusion, reactions, and dielectric relaxation terms are stiff relative to advection, and interact with each other strongly. The iterative time-stepping approach efficiently couples all the terms, and exhibits second-order convergence in space and time. The algorithm is amenable to one-, two- and three-dimensional applications, and has been implemented in the context of a block-structured adaptive mesh refinement framework. We will present details of the method and show examples of its performance on a range

of idealized and practical applications.

Valentina Ricchiuti
University of California Irvine, MAE Department
Lawrence Berkeley National Lab
vricchiuti@lbl.gov

Marc Day
Lawrence Berleley National Laboratories
MSDay@lbl.gov

CP2

Simulating Interactions of Detonation, Ionization Chemistry, and Magnetohydrodynamics

Oxyfuel combustion is a strategy to remove NOx emissions from combustion-based power generation. However, the resulting high temperatures incur material challenges for gas turbine technology. Detonation-driven flow through a magnetohydrodynamic (MHD) generator offers a potential solution by directly extracting power from conductive fluid flow via the Lorentz force, removing immersed moving components unable to withstand high temperatures. In addition, detonation cycles improve thermodynamic efficiency. Modeling these coupled systems requires the simultaneous consideration of compressible flow, chemical reactions, and magnetic field interaction. To tackle this challenge, a Riemann solver, implicit ordinary differential equation integrators, and a Galerkin finite-element solver are coupled to solve Euler's equations, stiff chemical kinetics equations, and decoupled Maxwell's equations. Each solver will first be verified and validated separately, and the coupled system validated with literature results and experimental data. Simulations of hydrogen and methane oxyfuel combustion will be performed over a range of conditions to determine power extraction and emissions. In addition, seed particles are typically necessary to increase the fluids electrical conductivity through ionization; the impact of seed composition and quantity will be assessed. Results will provide insight into the complex, and possibly adverse, interactions between detonation, ionization, and MHD effects.

Matthew F. Zaiger, David Blunck, Kyle E. Niemeyer
Oregon State University
zaigerm@oregonstate.edu, david.blunck@oregonstate.edu, Kyle.Niemeyer@oregonstate.edu

CP3

The Laminar Flamelet Model Combined with Collision Porosity Distance Algorithm Applied to Accidental Explosion Modelling

This work presents a novel implementation of the Porosity Distributed Resistance (PDR) model coupled with a structured 3D Navier-Stokes solver and Flamelet combustion model. The geometry is represented by porosities that are computed by calculating the minimum distance between two convex sets. The GilbertJohnsonKeerthi (GJK) distance algorithm is used to check the collision between an element of the mesh and an object of the geometrical model to calculate the mesh porosity (volume and area). The combustion model considers that the flame area increases with the intensity of the turbulence up to a maximum, after which reductions in the burning rate due to flame stretch decreases the flame area. The model has no dependence on the length scale of the turbulence. The only length scale is the laminar flamelet length scale which is a diffusive length scale associated with the internal structure and with the maximum curvature of the laminar flamelet. The main concept is to quantify the length scale of the flame uniquely for the turbulent flame, assuming that the turbulent flame will select its own wrinkling length scale in accordance with the perturbations from the turbulent velocity field ahead of the flame front. The modified Lax-Friedrichs scheme is applied in the finite volume formulation. The results of the simulation of initial phase of gas explosion are in accordance with the current understanding of accidental explosions.

Tatiele Ferreira
Faculty of Chemical Engineering - UNICAMP
tatieledf@gmail.com

Rogério Santos
Faculty of Mechanical Engineering - University of Campinas
roger7@fem.unicamp.br

Sávio Vianna
Faculty of Chemical Engineering - University of Campinas
savio@feq.unicamp.br

CP3

An RCCE-ANN Tabulation Approach Applied to Sydney Flame L

In this work, a tabulated mechanism for methane-air combustion via Rate-Controlled Constrained Equilibrium (RCCE) and Artificial Neural Networks (ANNs) is presented and applied to a highly extinguishing non-premixed turbulent flame from the Sydney burner. The objective of our methodology is to train the ANN architecture on an abstract problem and then simulate a real flame of the same fuel, the Sydney flame L. In the present case, an ensemble of laminar flamelets with random strain rates is being used to train the self-organized map (SOM) - Multilayer Perceptron (MLP) approach. In order to reduce the number of variables and assist the ANN training, the RCCE approach is applied on the GRI-1.2 detailed mechanism, reducing the chemical space dimensionality to 17 species. The flow field is resolved through Large Eddy Simulation (LES) method employing the Eulerian Stochastic Fields approach as a solution scheme for the transport equation of the sub grid Probability Density Function (PDF) of the reactive scalars. Results demonstrate reasonable agreement with experiments, whereas the SOM-MLP approach provides a representation of the flame within reasonable CPU times, employing modest computation resources.

Lucas Franke
Imperial College London
l.franke14@imperial.ac.uk

Stelios Rigopoulos
Imperial College London
Department of Mechanical Engineering
s.rigopoulos@imperial.ac.uk

CP3

Comparison of Differential Diffusion Flamelet Modeling Approaches in Turbulent Oxy-Fuel Flames

Differential diffusion is an important phenomenon, especially in oxy-fuel flames as experimentally shown by (Sevault et al., Combust. Flame 159, 2012). However, the interaction between turbulent and molecular diffusion is

not entirely understood now. Nevertheless, several models exist to incorporate differential diffusion into turbulent flame modeling. Based on the data of the turbulent oxy-fuel flame investigated in (Sevault et al., Combust. Flame 159, 2012), different diffusion modeling approaches in the context of flamelet modeling are investigated by means of a prior analysis and coupled LES. These models are: 1) equal diffusivity of all species (Lei=1) (N. Peters, Proc. Combust. Inst. 21, 1986), 2) differential diffusion of species (mixture averaged diffusion) (H. Pitsch, N. Peters, Combust. Flame 114, 1998) and 3) incorporate influence of turbulent mixing by performing a blending between the previous mentioned models (H. Wang, Phys. Fluids 28, 2016). As the results indicate, the pure models 1) and 2) are not able to reproduce the flame structure, whereas model 3) as a combination of 1) and 2) gives a much better agreement with experimental data. Nevertheless, discrepancies are still observable in some species, which can not be overcome by introducing only one parameter which represents the influence of turbulence. The importance of correct diffusion modeling is underlined by a coupled LES where error accumulation and propagation can be observed.

Sandro Gierth
TU Bergakademie Freiberg
IEC
sandro.gierth@iec.tu-freiberg.de

Franziska Hunger, Sebastian Popp
TU Bergakademie Freiberg
Numerical Thermo-Fluid Dynamics
franziska.hunger@iec.tu-freiberg.de,
sebastian.popp@iec.tu-freiberg.de

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

CP3

Portable Tabulation for Thermochemical and Radiation Properties in Combustion Simulations

Tabulation is common in combustion applications to reduce computational time by performing expensive calculations a priori and looking up tabulated results during the CFD simulation. We present two open-source libraries that perform tabulation of thermochemical properties as well as radiative properties. The thermochemical tabulation library (TabProps) supports one to five independent variables and a variety of thermochemical models including flame sheet, equilibrium (adiabatic and with heat loss), steady laminar flamelets, etc. The radiative properly library (RadProps) provides grey gas property calculations for reacting gas mixtures over a wide range of temperatures and compositions. These libraries support various order of interpolants based on Lagrange polynomials. In addition, derivative calculations are also provided to enable Jacobian information to be obtained from the tabulated quantities. Both libraries support CPU and GPU calculations. We present performance results for these libraries, showing significant speedups on GPU of up to 120x over serial CPU calculations for table retrieval.

Babak Goshayeshi
University of Utah
b.goshayeshi@gmail.com

James C. Sutherland
Department of Chemical Engineering
The University of Utah
james.sutherland@chemeng.utah.edu

CP3

Spectral Matrix Analysis of the Semi-Discrete Flamelet Equations

We use numerical eigensolvers to determine the spectra (sets of eigenvalues) of global discretization matrices representing the transient flamelet equations. We perform this analysis to gain insight on the nature and time scales of nonlinear coupling between diffusive transport and chemical kinetics. The flamelet equations allow precise control of diffusive time scales through the scalar dissipation rate, facilitating studies of matrix spectra through transient ignition and extinction phenomena whose understanding is crucial to the development of the advanced implicit methods and nonlinear solvers necessary for detailed kinetic models. Many methods stand to gain from this knowledge, such as operator splitting, spectral deferred correction, and advanced continuation methods for traditional monolithic implicit techniques.

Michael A. Hansen
University of Utah
Sandia National Laboratories
mike.hansen.utah@gmail.com

James C. Sutherland
Department of Chemical Engineering
The University of Utah
james.sutherland@chemeng.utah.edu

CP3

Assessment of Flamelet Tabulation Strategies for Pulverized Coal Combustion in a Strained Flow Configuration

Pulverized coal combustion is a technologically relevant process in industrial furnaces. Modelling this process is demanding due to multi-phase flow, heterogeneous reactions at particle surfaces and the structural complexity of coal in general. In this work, a flamelet modelling approach (FPV) is proposed that utilizes strained gaseous flamelets. As a reference case, a lean premixed methane-air stagnation flame with coal particle loading is investigated. The original setup has been proposed by Xia et al. [M. Xia, D. Zabrodiec, P. Scouflaire, B. Fiorina, N. Darabiha, Proc. Combust. Inst. (2016), in press], who also published experimental data. Firstly, a full chemistry solution is validated against the experiments and thereafter the boundary conditions are varied to examine different extents of char burnout. The flamelet model is assessed with an a-priori analysis, where the full chemistry solution is used for a look-up from the flamelet table. Furthermore, calculations with full coupling of the flamelet table (a-posteriori analysis) are performed and examined. In the assessment of the flamelet solutions, special attention is put on the cross-scalar dissipation rate, which can become important when conditioning on multiple composition space variables

(mixture fractions and progress variables).

Arne Scholtissek
TU Bergakademie Freiberg
TU Bergakademie Freiberg
arne.scholtissek@iec.tu-freiberg.de

Danny Messig
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
danny.messig@iec.tu-freiberg.de

Michele Vascellari
Virtuhcon, Chair of Numerical Thermo-Fluid Dynamics
TU Freiberg
Michele.Vascellari@vtc.tu-freiberg.de

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

CP4

DNS of An Autoigniting Air / N-Dodecane Temporal Jet at Diesel Engine Conditions

We present a direct numerical simulation of a turbulent autoigniting temporal jet between n-dodecane and diluted air at conditions representative of low temperature diesel engine combustion. In this simulation, the initial temperature and pressure conditions were carefully selected to result in a two-stage ignition event, in which low-temperature reactions play an important role during the ignition process. Reaction rates were computed using a 35-species reduced mechanism which included both the low- and high-temperature reactions pathways of n-dodecane. We focus our analysis on the mechanisms by which low-temperature reactions assist high-temperature ignition. Preliminary results indicate that ignition occurs at rich mixture compositions and that, differently from what has been observed in previous DNS studies of single-stage autoignition, the ignition delay time is shorter than the corresponding homogeneous ignition delay time. Our study reveals that, during the first stage of ignition, several cool flames appear within the lean regions of the jet and then quickly propagate towards those flow regions with richer mixture compositions, thus creating the conditions for hot ignition to occur. We provide a detail description of the mechanism by which the cool flame propagates in physical space, as well as of the flame propagation phase that follows localized autoignition.

Giulio Borghesi
Sandia National Laboratories
gborghe@sandia.gov

Jacqueline Chen
Combustion Research Facility
Sandia National Laboratories
jhchen@sandia.gov

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

CP4

Eulerian Simulation of Polydisperse Two-Phase Flame Propagation in a Turbulent Flow for a Large Range of Stokes Numbers

In two-phase turbulent combustion, the description of the spray phase plays an essential role because of the evaporation process that introduces a time lag for fuel availability and also because the spray distribution may not be homogeneous because of segregation effects induced by the turbulence. To describe this spray phase, Eulerian methods are here envisioned because of their great parallel efficiency and their ease of coupling with the gas phase compared to Lagrangian techniques. These methods have proven their capability to reproduce spray distribution in turbulent flows. In the present work, we propose to validate these moment methods in a reactive context, by investigating the ignition of a turbulent cloud of droplets. To describe the polydispersity as well as the droplet trajectory crossings inherent to turbulent flows, Two-Size Multifluid (TSM) moment method will be used in combination with the Anisotropic Gaussian model. Simulations will be performed with the AsphoMUSES solver. By covering a wide range of Stokes numbers, this work will provide a validity range for Eulerian methods for two-phase combustion.

Dennis Dunn, Macole Sabat, Jean Michel Dupays
Laboratoire EM2C
CNRS-CentraleSupélec
dennis.dunn@centralesupelec.fr,
macole.sabat@centralesupelec.fr,
jean-michel.dupays@centralesupelec.fr

Jorge César Brandle De Motta
CORIA
jorge.brandle@coria.fr

Aymeric Vié, Frédérique Laurent, Marc Massot
Laboratoire EM2C
CNRS-CentraleSupélec
aymeric.vie@centralesupelec.fr, frederique.laurent@centralesupelec.fr,
marc.massot@centralesupelec.fr

CP4

Coupled Eulerian-Lagrangian LES-pdf Simulation of a Combustion System with Full Resolution of the Primary Atomisation

A combustion system operating at ambient condition, previously studied experimentally by Rodrigues et al. [Combust. Flame 162 (2015), 759], is numerically simulated. The spray is injected through an industrial pressure swirl atomiser using liquid ethanol as fuel. The atomisation processes are simulated using a hybrid Eulerian-Lagrangian approach in which the fluid interface is resolved using a Volume-of-Fluid (VOF) method and liquid structures which become too small compared to the local mesh resolution are converted into Lagrangian point particles that are tracked based on the underlying flow. The evolution of the Lagrangian droplets in terms of evaporation and dispersion follow the stochastic particle approach to include the sub-grid-scale interactions. This allows for an accurate modelling of the primary atomisation region while maintaining affordable computational cost, since the interface dynamics of the small droplets are not resolved. The combustion simulation is performed in the context of Large Eddy Simulation (LES) and the transported pdf-equation for the scalars is solved using the stochastic fields approach. The results show that the velocity profiles of the droplets within their size classes as well as the integral particle size distribution, which is represented by the Sauter Mean Diameter (SMD), measured in the corresponding experiments

are accurately reproduced. The gas phase temperature and velocity are also in good agreement with the measurements.

Fabien Evrard, Simon Gallot-Lavallée, Fabian Denner, Berend van Wachem
Imperial College London
f.evrard13@imperial.ac.uk,
simon.gallot-lavallee@imperial.ac.uk,
f.denner09@imperial.ac.uk, b.van-wachem@imperial.ac.uk

William Jones
Department of Mechnical Engineering
Imperial College
w.jones@imperial.ac.uk

CP4

Numerical Investigation of the Stability of a Spray Oxyfuel Flame Diluted by Carbon Dioxide

The influence of CO_2 concentration on the characteristics of spray flames is studied. It is common practice to adopt this technique to comply with the regulations on NO_x production. A numerical investigation using Large Eddy Simulation where combustion is modelled using the pdf approach with scalar field solved by the stochastic fields method is presented. In addition, the dispersed phase is simulated using the Lagrangian point particle approach and a conditional injection method is employed. A lab-scale experiment by Cléon et al. (2015) is selected to validate the results both for the dispersed and continuous phases. Three different CO_2 dilution ratios are considered. The comparison of the velocity fields and correlation of droplet size-velocity is promising for all cases. It is observed that the flame structures for the three cases reveal substantial differences in the lift-off and reaction zones. Similar flame characteristics were also observed experimentally where an increased volume fraction of CO_2 leads to a higher lift-off height and the presence of a double flame structure. At a lower CO_2 concentration, the flame is anchored in the region close to the nozzle. CO produced by the flame is also simulated and compared with the experimental data to understand the correlation with the flame characteristics. This work provides further insight in the analysis of the flames considered together with a satisfactory agreement with the experimental results.

Simon Gallot-Lavallée, Dongwon Noh, Andrew Marquis
Imperial College London
simon.gallot-lavallee@imperial.ac.uk,
dongwon.noh10@imperial.ac.uk,
a.marquis@imperial.ac.uk

William Jones
Department of Mechnical Engineering
Imperial College
w.jones@imperial.ac.uk

CP4

Analysis and Regimes of Multicomponent Spray Combustion Using DNS

To examine the effect of multicomponent transportation fuels on the evaporation and combustion, direct numerical simulations of a turbulent counterflow spray flame configuration are performed under consideration of preferential evaporation and combustion of a multicomponent surrogate fuel. The simulation involves using accurate models for multicomponent droplet evaporation and appropriately reduced mechanisms for the combustion in the gaseous carrier phase. While previous work focused on the role of preferential evaporation on the combustion in a homogenous environment, this studies examines the role of droplet clusters and turbulent mixing on the evaporation and low-temperature ignition behavior. Results are compared against 0D batch-reactor simulations. Analysis is performed to demarcate relevant combustion regimes for multicomponent spray-flames, introducing additional timescales arising from the competition between preferential evaporation, turbulence and reaction chemistry.

Pavan B. Govindaraju
Stanford University
pavang@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP4

Modeling N-Dodecane Spray Combustion with a Representative Interactive Linear Eddy Model

Many new combustion concepts are currently being investigated to improve engines in terms of both efficiency and emissions. Examples include homogeneous charge compression ignition (HCCI), lean stratified premixed combustion, stratified charge compression ignition (SCCI), and high levels of exhaust gas recirculation (EGR) in diesel engines, known as low temperature combustion (LTC). Typical combustion temperatures in all of these combustion concepts have in common that the temperatures are lower than in traditional engines. To further improve and develop combustion concepts for clean and highly efficient engines, it is necessary to develop new computational tools that can be used to describe and optimize processes in non-standard conditions, such as low temperature combustion. Thus, in the presented study a recently developed model (RILEM: Representative Interactive Linear Eddy Model) for modeling non-premixed combustion, regime-independently, was used to simulate the so called Spray B, a heavy-duty optical engine experiment that was performed within the Engine Combustion Network (ECN) . The RILEM directly resolves the influence of the mixing on the chemistry, or turbulence-chemistry interactions, through stochastic sequences of statically independent eddy events. Cylinder pressure, heat release rates, ignition delay time and flame lift-off from the computation are compared to experiments under parametric variation of temperatures at different oxygen contents.

Tim Lackmann
Chalmers University of Technology
tim.lackmann@chalmers.se

Tommaso Lucchini, Gianluca D'Errico
Politecnico di Milano
tommaso.lucchini@polimi.it, gianluca.derrico@polimi.it

Alan Kerstein
Consultant
alan.kerstein@gmail.com

Michael Oevermann
Chalmers University of Technology

michael.oevermann@chalmers.se

CP5

Linear Stability Analysis of Detonation Waves with Realistic Chemical Kinetic Schemes

The normal-mode, linear stability of the one-dimensional, Zeldovich-von-Neumann-Doring (ZND) detonation solution yields information about the behaviour of multi-dimensional, detonation dynamics. The stability of detonation models has been explored in the last 20 years with increasingly more complex chemical kinetic schemes, though such schemes are still simple when compared to real chemical kinetics. We approach here the detonation stability problem using realistic chemical kinetic schemes. The stability problem is solved using a pseudo-spectral method. One hurdle, when solving this problem lies in finding a suitable, independent variable. So far, the problem has mostly been expressed as a function of physical space or of a reaction progress variable, normally a mixture component mass fraction λ_i. In the first case, limitations arise for simple, Arrhenius kinetic schemes, when the reaction zone is unbounded, while the second case is limited when schemes with several reactions have all component mass fractions with $d\lambda_i/dx$ somewhere in the reaction zone. We circumvent this limitation by using particle velocity as an independent velocity for kinetic schemes composed of only strictly exothermic steps and by considering entropy, the true reaction progress variable, for more complex schemes. Only ideal gas equations of state are considered so far.

Charles B. Kiyanda
Concordia University, Montreal, Canada
kiyanda@encs.concordia.ca

Mark Short
Los Alamos National Laboratory
short1@lanl.gov

CP5

The Role of Darrieus-Landau Instability on Turbulent Premixed Flame Propagation

The effects of Darrieus-Landau (DL) or hydrodynamic instability on flame propagation is investigated numerically for turbulent premixed flames in a Bunsen configuration. Recent experiments on air/propane Bunsen flames have shown that by varying the equivalence ratio and/or the Bunsen diameter the DL instability can be induced or suppressed. Similarly, in numerical simulations, the instabilities are triggered by varying the ratio between the flame thickness and a representative hydrodynamic length, prompting a dramatic morphological effect on the flame and a relative increase in turbulent propagation speed. Simulations are carried out using a deficient reactant approach in the low-Mach limit, implemented in the highly scalable spectral element code nek5000. The deficient reactant model is coherent with results from asymptotic theory thus allowing stability limits to be known unambiguously. The spectral element method yields minimal numerical diffusion and dispersion, allowing a detailed characterization of flame morphology and contributions to stretch. The latter is analyzed and statistically related to the flame curvature while the skewness of the curvature distribution is found to be a consistent instability marker.

Pasquale Lapenna, Rachele Lamioni
University of Rome La Sapienza
pasquale.lapenna@uniroma1.it,
rachele.lamioni@uniroma1.it

Francesco Creta
University of Rome, La Sapienza
Department of Mechanics and Aeronautics
Francesco.Creta@uniroma1.it

Guido Troiani
ENEA C.R. Casaccia
guido.troiani@enea.it

CP5

Accuracy and Stability of Finite Differences in Premixed Combustion DNS

Filtering is often used in high fidelity simulations of compressible reacting flows. The filtering is introduced to counter oscillations thought to be caused by under-resolution or numerical boundary schemes. This presentation outlines the role of flame induced heat release on the stability of Direct Numerical Simulations. The effects of heat release are examined via an imposed flame profile in a much simplified one-dimensional model problem, which is then spatially discretized using commonly employed finite differences. Schemes that are *Left Half Plane* (LHP) stable for non-reacting flows are found to lose this property in the presence of temperature gradients; it is this loss of stability that requires correction via filtering or damping through diffusive terms. The root cause of the destabilization is traced back to the discretization schemes capacity (or otherwise) to satisfy integration by parts. This observation, in conjunction with an application of the Lyapunov equation, then provides guidance for schemes which remain either absolutely or conditionally stable with respect to heat release. Examples are provided for one dimensional laminar flames.

Robert Prosser
Dept of Mechanical, Aerospace and Civil Engineering, University of Manchester
robert.prosser@manchester.ac.uk

CP5

Nonlinear Frequency Response Analysis of Laminar Premixed Flames

The stretched laminar flamelet model provides a convenient approach to embed local realistic chemical kinetics when simulating turbulent premixed flames. The significance of the transient aspects of strained flamelet models has been discussed in the literature with assertions that their chemical time scales are sufficiently short compared to the turbulent time scales. Less discussed is the unsteady motion of a curved flame front component of stretch rate. A model developed and validated for use with transient premixed flame dynamics in a cylindrically-symmetric geometry was applied to study flame response when the flow and scalar fields remain aligned (i.e., no strain). The model is applied to conditions where the flame expands (positive stretch) and contracts (negative stretch) radially. This analysis suggests that laminar premixed flames do not always approach the equilibrium unstretched structure as rapidly as the flamelet model time scales imply, especially for lean premixed conditions. The addition of the externally-defined oscillating mass flow rate changes the dynamics of the flame due to a changing stretch rate. Tracking such changes in the flame dynamics with full chemistry requires considerable computational effort. Therefore, a frequency response analysis was applied as a

process characterization tool to study the flame dynamics and unravel its complex non-linear processes using graphical and analytical tools (transfer functions).

Meysam Sahafzadeh
Ryerson University
meysam.sahafzadeh@ryerson.ca

Larry Kostiuk
University of Alberta
Edmonton, Alberta, Canada
lkostiuk@ualberta.ca

Seth Dworkin
Ryerson University
seth.dworkin@ryerson.ca

CP5

Flame Stabilisation and Dynamics in a Sequential Combustor at Atmospheric and High Pressure

The flame anchored in a sequential combustor fed by vitiated air is investigated in this numerical study. The flame stabilization mechanisms and the flame response to temperature perturbations are studied at 1 and 10 bar using LES with Analytically Reduced Chemistry. The simulated domain is the second stage of a sequential combustor concept with methane injected into hot vitiated cross flow supplied from a first stage lean swirled flame.
Results show that an increase of pressure P changes the dominant stabilization mechanism from mainly propagation-driven to pure autoignition. The transition between the two is mapped over a wide range of unburned gas temperature and P. Although both flames qualitatively look similar they are subject to very different combustion processes.
The flame response to inlet temperature modulation T' is also investigated. It is shown that small T' induce large amplitude heat release rate HRR response. This is because, for most of the conditions investigated, the main reaction zone is highly perturbed by autoignition kernels developing upstream in the mixing zone. In contrast to conventional swirled-turbulent flames, which often feature a monotonic decrease of the flame describing function gain when the acoustic perturbation amplitude is increased, the HRR response of the present flame can increase beyond a certain amplitude of T'. This indicates that these flames could be prone to triggering mechanisms due to inlet temperature perturbations.

Oliver Schulz
CAPS Laboratory
Department of Mechanical and Process Engineering
oschulz@ethz.ch

Nicolas Noiray
CAPS Laboratory
Department of Mechanical and Process Engineering, ETH Zurich
noirayn@ethz.ch

CP5

Thermoacoustics of Annular Combustors

The aim of the present work is to predict the unsteady behaviour of an 18-burner annular combustor in response to acoustic excitation. Computational Fluid Dynamics simulations using both URANS and LES modelling have been carried out to capture the fully-coupled thermoacoustic interactions in the chamber. Acoustic instabilities in lean premixed annular combustors can cause high-amplitude pressure fluctuations. Resulting variations in the heat release rate may also lead to self-sustained acoustic oscillations. It is thus essential to be able to predict the effect of instabilities on a new combustor design. The work uses experimental data from an 18-burner annular combustor rig built in the Cambridge University Engineering Department. Computer-aided Design work for a complete representation of the exact rig model has been completed. Geometry repair has been undertaken and meshing has been applied for variants of the complex geometry from single to 18-burner configurations. Initial single burner analyses concerned with the choice of turbulence model have also been performed. A reacting swirling flow study has been conducted on the single burner model. Other single and multiple-burner investigations are in progress which will include acoustically forced oscillating reacting flows, leading up to LES of the full 18-burner configuration.

Audrey Valreau, Chin Yik Lee, Stewart Cant
University of Cambridge
aslv2@cam.ac.uk, cyl36@cam.ac.uk, rsc10@cam.ac.uk

CP6

A Web-Based Tool for Simulation and Numerical Analysis of Zero-Dimensional Combustion Problems

Zero-dimensional reactors isolate chemistry from mixing and transport effects, enabling their usage in a variety of applications from chemical mechanism development and validation of basic combustion models for more complex flame simulation. These models isolate not only the chemistry of combustion, but also the complex numerical difficulties of the chemistry. Analysis of the chemical source Jacobian provides insight towards reduced mechanisms and improved numerical methods. This talk presents a web-based application for simulation and analysis of zero-dimensional systems, which can generate transient and/or steady state solutions for a wide range of mechanisms using a very robust time integration scheme. The web-based application also provides support for post-processing the results to obtain transient eigenvalue and explosive mode analysis. We briefly review the theory of the application as well as the time integration scheme and present results for a variety of mechanisms.

Elizabeth Armstrong, Michael Hansen
University of Utah
elizabeth.armstrong@chemeng.utah.edu,
mike.hansen@chemeng.utah.edu

James C. Sutherland
Department of Chemical Engineering
The University of Utah
james.sutherland@chemeng.utah.edu

CP6

The First Investigation of the Hamish Code: An Adaptive Mesh Solver for Turbulent Reacting Flows

The Hamish code has been recently developed in the Department of Engineering, University of Cambridge to carry out direct numerical and large-eddy simulations of turbulent reacting flows. An unstructured adaptive mesh refinement (AMR)-based finite-volume method is adopted to resolve the fine flow structures presented in combustion

processes. The AMR data structure is built by the combination of the Morton code space filling method and the Octree algorithm, which allows the code to have a good parallel performance. The Hamish code was respectively assessed for the Taylor-Green vortex (TGV) case using a static mesh and a thermal diffusion problem using a dynamically refined mesh. The assessments show that good accuracy is observed in computing the kinetic energy and resolving vorticity for the TGV case. The scalability of the code is also assessed and a linear speedup is obtained up to 512 processors of a NextScale cluster for the TGV case using 1283 cells. In the thermal diffusion test case, a clear advantage of using AMR is observed, compared to only a static mesh. Fewer cells are needed and higher resolution of the flame front is obtained when the mesh is dynamically generated. The current version of Hamish will be further optimised to improve its performance.

Jian Fang, Charles Moulinec
Daresbury Laboratory
Science and Technology Facilities Council
jian.fang@stfc.ac.uk, charles.moulinec@stfc.ac.uk

David Emerson
Scientific Computing Department STFC Daresbury Laboratory
david.emerson@stfc.ac.uk

Nilanjan Chakraborty
Newcastle University
nilanjan.chakraborty@newcastle.ac.uk

Stewart Cant
University of Cambridge
stewart.cant@eng.cam.ac.uk

CP6

Numerical Simulation of Transcritical H2/O2 Flame

Combustion in liquid rocket engines (LRE) happens under severe thermodynamical conditions: pressure exceeds the critical pressure of injected propellants and temperature is cryogenic. Such a situation requires an important effort of modeling: real gas effects are incorporated through cubic equations of state along with pressure-correction terms, and transport properties follow specific rules. Modeling for turbulent combustion is also an issue. To assess the validity of future turbulent combustion models, a two-dimensional direct numerical simulation is performed using the numerical solver SiTCom-B (https://www.coria-cfd.fr/index.php/SiTCom-B). This benchmark corresponds to a splitter-plate configuration separating a cryogenic flow of liquid oxygen from a gaseous flow of hydrogen. Both fluids experience a pressure level of 10.0 MPa. Classical geometrical and incoming flow characteristics encountered in LRE are used. A detailed chemistry containing 8 reacting species and 21 elementary reactions is considered to model the oxy-combustion of hydrogen. The impact of surface tension effects is assessed through a diffuse interface approach that is based on the second gradient theory.

Umut Guven
CORIA UMR CNRS 6614
umut.guven@insa-rouen.fr

Guillaume Ribert
CORIA - CNRS UMR6614
INSA de Rouen
ribert@coria.fr

CP6

Numerical Methods for Transcritical Real-Fluid Reacting Flows Using the Flamelet Progress Variable Approach

A finite volume method with tabulated chemistry is developed for simulating the turbulent reacting flows at transcritical conditions. Spurious pressure oscillations associated with fully conservative formulations are addressed by extending a double-flux model to real-fluid conditions. The flamelet progress variable (FPV) approach is extended to be applied in consistence with the real-fluid equation of state. An entropy-stable scheme that combines high-order non-dissipative and low-order dissipative finite-volume schemes is proposed to preserve the physical realizability of numerical solutions across large density gradients. The resulting method is applied to a series of test cases to demonstrate the capability in simulations of problems that are relevant for multi-species transcritical real-fluid reacting flows.

Peter C. Ma, Yu Lv
Stanford University
peterma@stanford.edu, ylv@stanford.edu

Daniel Banuti
Stanford University
Center for Turbulence Research
dbanuti@stanford.edu

Jean-Pierre Hickey
University of Waterloo
jean-pierre.hickey@uwaterloo.ca

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP6

Identification of Low-Dimensional Manifolds in Coal Combustion

Previous studies have shown that PCA is an effective means of identifying low dimensional manifolds within the thermochemical state space of turbulent combustion systems, but to date, the application of PCA in the scope of combustion has been limited to homogeneous gas-phase systems. This talk applies PCA to coal combustion to identify low-dimensional manifolds and generate models for the thermochemical state variables as functions of the principal components. We demonstrate that low-dimensional manifolds can be identified within the state space of a turbulent coal combustion system for both gas and particle phase variables using PCA. The results indicate that PCA can be used to adequately parameterize gas and particle phase variables when used in conjunction with a nonlinear regression technique.

Josh T. Mcconnell
University of Utah
Dept. of Chemical Engineering
josh.mcconnell@chemeng.utah.edu

James C. Sutherland

Department of Chemical Engineering
The University of Utah
james.sutherland@chemeng.utah.edu

CP6

Transported PDF Modeling of Turbulent Flames Using the Flamelet Generated Manifold Chemistry Model

Numerical simulations of turbulent combustion using detailed reaction mechanism are computationally expensive. To reduce the computational cost, tabulated chemistry methods such as the ?amelet generated manifold (FGM) method have been developed. In the FGM method the chemistry is reduced to the mixture fraction (a non-reacting scalar) and progress variable (a reacting scalar). For turbulent flames the FGM method is commonly combined with a presumed-shape PDF approach in which mixture fraction and progress variable are assumed to be independent. In this work we will detail the methodology to account for turbulence-chemistry interaction by solving the composition probability density function (PDF) transport equation with a Lagrangian Monte Carlo method. The proposed FGM/PDF method is implemented in the open source CFD code OpenFOAM. We will investigate the accuracy of the FGM method by comparing predictions for Sandia flames D & E based on a FGM table and based on a detailed chemical mechanism (DRM22) with available experimental results. To enable a comparison, the FGM table is based on non-premixed flamelet solutions using the same DRM22 chemical mechanism.

Michael Stoellinger
University of Wyoming
Department of Mathematics
mstoell@uwyo.edu

Vasu Jaganath
University of Wyoming
Department of MEchanical Engineering
vjagana1@uwyo.edu

CP7

Modeling of Isolated Droplet Combustion of Sooting Fuels Under Microgravity Environment

Microgravity droplet combustion offers unique platform to study the sooting characteristics of single and multi-component real fuels. The spherically symmetric droplet burning configuration incorporates many important combustion aspects including moving boundary effect, detailed chemistry, soot formation and oxidation, radiative transport and temperature dependent variable properties. In this numerical study, a recently developed 1-D multi-component droplet combustion model capable of incorporating comprehensive kinetics and spectrally dependent radiation scheme has been utilized to analyze the sooting behavior of isolated droplets of ethanol (C2H5OH), n-heptane (n-C7H16) and primary reference fuel (PRF). A semi-detailed phenomenological soot model is incorporated within the existing droplet combustion code. Model predictions of droplet regression history, flame stand-off ratio (Df / Dd) and soot-shell stand-off ratio (Ds / Dd) are compared against the micro or reduced gravity droplet combustion experimental results of ethanol, n-heptane and PRF blends available in the literature. Finally, the detailed flame structure of such sooting fuels are analyzed to comprehend the influence of soot on the overall droplet combustion behavior.

Fahd E. Alam
Department of Mechanical Engineering, University of South
Carolina, Columbia, SC
alamme@email.sc.edu

Frederick L. Dryer
Mechanical and Aerospace Engineering, Princeton University,
Princeton, NJ, USA
fldryer@princeton.edu

Tanvir I. Farouk
Mechanical Engineering, University of South Carolina,
Columbia, SC, USA
tfarouk@sc.edu

CP7

Droplet Formation and Recognition: A Droplet Tracking Algorithm for Primary Breakup Modelling

In this study, we conduct numerical simulations of spray formation through air-blasted liquid-sheet breakup to investigate the formation and characteristics of liquid droplets. The Robust Conservative Level Set (RCLS) method, coupled with high-order WENO treatment of the level-set transport equation, is used to capture the motion and topological changes of the liquid-sheet, and the primary breakup process. The need for droplet detection and transfer arises from the computational modelling of atomisation, which generally involves two stages: primary breakup where drops are detaching from the liquid core and secondary breakup where the droplets produced at the previous stage further disintegrate into smaller droplets. The faithful prediction of the spray requires the simulation of both primary and secondary breakup. In this work, primary breakup is modelled intrinsically using the interface-capturing method RCLS. The droplets generated are then identified, removed from the level-set formulation, and stored for further analysis including the calculation of geometrical and physical parameters. This strategy further allows the modelling capability to export these droplets as boundary conditions into a Lagrangian tracking framework, equipped with an appropriate secondary breakup model, to simulate the final fine spray formation, prior to spray combustion modelling.

Camille Bilger, Stewart Cant
University of Cambridge
cb757@cam.ac.uk, rsc10@cam.ac.uk

CP7

Conjugate Heat Transfer Modeling in a Kerosene/Air Spray Flame Impacting a Plate. Application to Fire Resistance on Helicopter Crankcases

Airworthiness standards require a fire resistance demonstration for aircraft or helicopter engines to obtain a type certificate. This demonstration relies on tests performed with prototype engines in the late stages of the development. In these tests, a standardized flame with imposed temperature and heat flux is placed next to the engine casing during a given time. The aim of this work is to provide a better characterization of a kerosene/air certification burner in order to reach a better understanding of

the thermal environment during fire tests. To this purpose, Large-Eddy Simulation of the certification burner is carried out. Spray combustion, forced convection on walls, conduction in the solid parts of the burner and radiation of burnt gases are coupled to achieve a detailed description of heat transfer. Simulations are performed on unstructured grids with 40 million tetrahedral cells, using the finite-volume YALES2 code. The spray is modeled with a point-particle Lagrangian approach and the injection parameters are obtained from dedicated experimental measurements. The LES model is finally applied to the prediction of heat transfer in a flame impaction configuration. A well instrumented metal plate is here investigated as a simplified test case. Experimental and numerical results such as temperature and heat flux distributions are compared and discussed. To a large extent, the aim is to progress on fire test modelling so as to minimize the risks of test failure.

Lancelot Boulet
CNRS UMR 6614 - CORIA
lancelot.boulet@coria.fr

Pierre Bénard
CORIA - CNRS UMR6614, Université et INSA de Rouen
pierre.benard@coria.fr

Ghislain Lartigue
CORIA - CNRS UMR6614
ghislain.lartigue@coria.fr

Vincent R. Moureau
CORIA Laboratory - CNRS UMR6614
Université et INSA de Rouen
vincent.moureau@coria.fr

Sheddia Didorally
Safran Helicopter Engines
sheddia.didorally@safrangroup.com

CP7

Counter-Flow Spray Pulsated Flames: From Experimental Measurements to Numerical Simulation

The scope of the present contribution is to investigate a configuration of stationary and pulsated counterflow polydisperse sprays flames, where the pulsation mechanism does not involve or excite any acoustic mode. First an original experimental set up is proposed fulfilling these specifications, as well as some new diagnostics and data analysis tools in order to improve the time and space resolution. This is especially important in order to propose a set of detailed quantitative comparisons with high-fidelity numerical simulations. These numerical simulations rely on both a Lagrangian and Eulerian multi-fluid models able to describe accurately polydisperse sprays in a multi-species reacting gaseous flow field modeled using the low Mach number limit of the Navier-Stokes equations. We use an in-house code AsphoMUSES with realizable, robust and accurate numerical methods in order to conduct direct numerical simulations of the proposed configurations, relying on detailed boundary conditions provided by the experimental measurements. We present quantitative comparisons between experimental measurements and simulations and prove that the proposed Eulerian approach is able to capture the two-way coupling of the gas-spray interactions as well as combustion dynamics. Such a configuration is also intended to become a reference set of solution in order to validate industrial code, as well as their models and numerical methods for spray and gas resolution.

Jorge Cesar Brandle De Motta
Coria, Université de Rouen
jorge.brandle@coria.fr

Dennis Dunn
EM2C, CentraleSupélec
dennis.dunn@ecp.fr

Matthieu Boileau
IRMA, Université Strasbourg
matthieu.boileau@math.unistra.fr

Laurent Zimmer, Benjamin Robbes
EM2C, CentraleSupélec
laurent.zimmer@centralesupelec.fr,
benjamin.robbes@centralesupelec.fr

Eleonore Riber, Bénédicte Cuenot
CERFACS
eleonore.riber@cerfacs.fr, cuenot@cerfacs.fr

Julien Réveillon
CORIA, Université de Rouen
julien.reveillon@coria.fr

Frédérique Laurent-Nègre
EM2C, CentraleSupélec
frederic.laurent@em2c.ecp.fr

Marc Massot
Laboratoire EM2C
CNRS-CentraleSupélec
marc.massot@centralesupelec.fr

CP7

A Filtered Tabulated Chemistry Model for LES of Spray Combustion

The proposed study focuses on LES of two-phase reactive flows using tabulated chemistry. For that purpose, the Filtered TAbulated Chemistry for LES (F-TACLES) is applied for the first time in a spray combustion context. A look-up table is first generated using filtered flamelet archetypes. Then the ability of the methodology to capture the propagation of 1-D filtered spray flames is addressed for different conditions of spray injection such as variation of droplet diameter and particle number density. The model is applied to the 3-D LES of a turbulent spray flame. The retained experiment, measured at CORIA laboratory, France, is a bluff-body burner operated at atmospheric pressure where the n-heptane spray is injected as a hollow cone in a coflow of air. Comparisons between experimental data and simulations for both reacting and non-reacting conditions are performed to assess the ability of the tabulated method and the LES flow solver to correctly predict the dynamics of the gaseous and liquid phases, especially the heat release rate distribution and the particles' position, velocity and temperature. The performances of the model to recover several key features of the turbulent flame, such as the lift-off height, are discussed.

Adrien Chatelier
ONERA
Laboratoire EM2C, CNRS, CentraleSupélec, U. Paris-Saclay
adrien.chatelier@centralesupelec.fr

Nasser Darabiha
Laboratoire EM2C
CNRS-CentraleSupélec
nasser.darabiha@centralesupelec.fr

Nicolas Bertier
ONERA
nicolas.bertier@onera.fr

Benoit Fiorina
Laboratoire EM2C, Ecole Centrale Paris
benoit.fiorina@centralesupelec.fr

CP7

Large-Eddy Simulation of Light-Round in an Annular Combustor Equipped with N-Heptane Spray Injectors

A combined experimental and numerical study of light-round under perfectly premixed conditions has previously demonstrated the ability of large-eddy simulation (LES) to predict such ignition process in a complex geometry using massively parallel computations. The present investigation aims at targeting a configuration closer to real applications by considering liquid n-heptane injection. The large-eddy simulation of the ignition sequence of a laboratory scale annular combustion chamber comprising sixteen swirled two-phase injectors is carried out with i) a mono-disperse Eulerian approach for the description of the liquid phase and ii) the thickened flame model with reduced chemistry for the reactive gaseous phase. The objective is first to assess this modeling approach to describe the two-phase reactive flow during the light-round before considering more advanced methods in the future. The simulation results are compared in terms of flame topology and light-round duration to the corresponding experimental high-speed images of the flame front propagation. Finally, analysis of the numerical results enables to characterize the different phenomena involved in the flame propagation. Similarly to previously investigated premixed conditions, the analysis highlights the influence of gas volumetric expansion on the absolute turbulent burning velocity during the spray flame propagation from burner to burner.

Thea Lancien
EM2C Laboratory, CNRS
thea.lancien@ecp.fr

Kevin Prieur
SAFRAN Tech, E&P
kevin.prieur@ecp.fr

Daniel Durox
EM2C, CNRS, Ecole Centrale Paris
daniel.durox@ecp.fr

Sebastien Candel
EM2C Laboratory, CNRS, CentraleSupelec
sebastien.candel@ecp.fr

Ronan Vicquelin
EM2C, CNRS, Ecole Centrale Paris
ronan.vicquelin@centralesupelec.fr

CP8

Scaling of Sooting Laminar Coflow Flames at Elevated Pressures: A New Appraoch

Soot is formed as a result of combustion of a fossil fuel under rich conditions or fuel pyrolysis. Laminar coflow diffusion flames are often used to study soot formation at elevated pressures due to their well-characterized configuration. Experimental studies of coflow laminar flames are typically conducted at a constant mass flow rate (constant Reynolds number) at increasing pressures. A numerical simulation of coflow laminar sooting flame at pressures ranging from 1 to 8 atm was performed at constant mass flow rate. The study clearly showed that, due to the effect of gravity, the flame shape changes as pressure is increased and as a result, the mixing field changes, which in return has a great effect on soot formation. In this work, a novel scaling approach of the flame at different pressures is explored. In this approach, both the Reynolds and Grashof's numbers are kept constant so that the effect of gravity is the same at all pressures. In order to keep the Grashof number constant, the diameter of the nozzle is modified as pressure varies. We report both numerical and experimental data proving that this approach guarantees the same non dimensional flow fields over a broad range of pressures. In the range of conditions studied, the Damkoehler number, which varies when both Reynolds and Grashof's numbers are kept constant, is shown to play a minor role. Hence, a set of suitable flames for investigating soot formation at pressure is identified.

Ahmed Abdelgadir
King Abdullah University Of Science and Technology (KAUST)
Clean Combustion Research Center (CCRC)
ahmed.abdelgadir@kaust.edu.sa

Scott Steinmetz
King Abdullah University of Science and Technology (KAUST)
Clean Combustion Research Center (CCRC)
scott.steinmetz@kaust.edu.sa

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Fabrizio Bisetti
University of Texas at Austin, USA
fbisetti@utexas.edu

William Roberts
King Abdullah University Of Science and Technology (KAUST)
Clean Combustion Research Center (CCRC)
william.roberts@kaust.edu.sa

CP8

Development of a Soot Particle Concentration Estimation Library for Industrial Combustion Applications

Soot emissions from combustion devices are known to have harmful effects on the environment and human health. As the transportation industry continues to expand, the development of techniques to reduce soot emissions remains a significant goal of researchers and industry. The complex geometries of engines and gas turbines make it computationally intractable to include detailed and accurate soot models in CFD simulations. This study leverages existing knowledge in soot modelling and soot formation fun-

damentals to advance the development of a stand-alone, computationally inexpensive soot concentration estimator to be linked to CFD simulations as a post-processor. The estimator consists of a library generated using the Lagrangian histories of soot-containing fluid parcels, which can then be used to predict soot concentration based on a pre-populated library. Updated results presented herein indicate the estimator shows potential for predicting peak soot volume fractions and soot emissions in laminar coflow diffusion flames in atmospheric and high pressure conditions. Results also show that as more flame data is added to the library to increase its accuracy, the predictive capabilities of the estimator become broader.

Raymond Alexander, Seth Dworkin
Ryerson University
raymond.alexander@ryerson.ca, seth.dworkin@ryerson.ca

CP8

Numerical Simulation of Soot Formation in Diffusion Flames

The world has a dependency on many different combustion devices for a variety of applications to meet the needs of modern society. However, this dependency has a negative effect in that the use of these devices ultimately results in greenhouse gas emissions, thereby further polluting the Earth. For this reason, combustion research is critical to give insight on how to better design these systems to minimize the harmful effects. Numerical simulation modelling of turbulent diffusion flames is still improving as it is not purely analytic, but rather in a semi-empirical state currently. This area of research involves the use of in-house combustion CFD codes to provide detailed analyses. This allows for modifications to be made to the code in order to test the results of proposed soot growth mechanisms. Through this methodology, numerical results can be compared to experimental data to determine whether or not these proposed mechanisms have some validity. In recent literature, results have shown that nascent soot can be rich in aliphatics and that soot can undergo mass growth in the absence of gas phase hydrogen atoms. For this reason, it is proposed that addition of aliphatic physical coagulation through collisions with soot may better characterize the mass growth of soot.

Nemanja Ceranic, Seth Dworkin
Ryerson University
nemanja.ceranic@ryerson.ca, seth.dworkin@ryerson.ca

CP8

Comparison of Moments-Based Approaches for Modeling Soot Population in Turbulent Flows

Representation of soot population is an important component in the computational prediction of particulate emissions. It is now accepted that moments-based approaches provide the most cost-effective implementation. However, there are a number of moments-based, multi-variate techniques with different levels of numerical complexity. In the past, development of such methods have been principally carried out on canonical laminar and 0-D flows. However, their applications in realistic solvers developed for turbulent combustion may face challenges. In this work, the relative computational expense of three common methods, CQMOM (Conditional Quadrature), HMOM (Hybrid), and ECQMOM (Extended Conditional Quadrature), are tested in a canonical turbulent flame. The Sandia ethylene jet flame configuration is chosen as the baseline test case with the KAUST high-pressure burner considered, using a similar flow configuration but higher operating pressure. Large eddy simulation (LES) is used as the turbulence modeling framework. In grid-filtered LES, the interaction of numerical and modeling errors is a first-order problem, which can seriously undermine the accuracy of computational results. In the past, special moments-based methods for solvers that transport high frequency content fluid have been developed. A similar analysis is carried out for the three soot modeling approaches above. Specifically, realizability of moments methods with nonlinear advection schemes will be discussed.

Shao Teng Chong, Venkat Raman
University of Michigan
stchong@umich.edu, ramanvr@umich.edu

Paul Arias
University of Michigan, Ann Arbor
pgarias@umich.edu

Hong Im
King Abdullah University of Science and Technology
hong.im@kaust.edu.sa

CP8

A Multi-Variate Sectional Method for the Description of Soot Production in Large Eddy Simulation

Soot control is an urgent societal issue and a political and industrial priority, due to its harmful impact on humans and environment. Soot production is a complex phenomenon governed by collisional and chemical processes that depend on the local properties of the gaseous phase, the flow and the particle size distribution (PSD). These processes lead to the emission of a population of solid particles of different sizes and morphology, classically characterized by its PSD. As a consequence, in order to correctly predict the total soot emission, a correct prediction of the evolution of the PSD is necessary. For this, sectional methods, based on a discretization of the PSD in different sub-intervals of size, represent a promising alternative to obtain an accurate description of the PSD. Only recently, they have been recently applied to Large Eddy Simulations of turbulent flames. In this work, a multi-variate extension of the sectional method to account for the fractal nature of soot particles is proposed to improve its accuracy on the PSD prediction. Results from the mono-variate and multi-variate formulations are compared on laminar flames in order to identify the best compromise between computational cost and results accuracy. The impact of a mono- or multi-variate description is finally evaluated by comparing results on soot volume fraction in a Large Eddy Simulation of a turbulent flame.

Benedetta G. Franzelli
Ecole Centrale Paris, EM2C CNRS UPR-288
benedetta.franzelli@ecp.fr

Aymeric Vié, Nasser Darabiha
Laboratoire EM2C
CNRS-CentraleSupélec
aymeric.vie@centralesupelec.fr,
nasser.darabiha@centralesupelec.fr

CP8

Monte Carlo Simulation of Particle Formation in

Premixed Flames Using a Detailed Soot Model

A very detailed soot model has been developed by D'Anna and coworkers. It describes soot formation, growth, oxidation, fragmentation and dehydrogenation with a quadvariate population balance equation (PBE). Each entity of the population is characterized by its type (large PAH, cluster or agglomerate), its state (stable or radical), its number of carbon atoms and its hydrogen/carbon ratio. The model has been applied in several studies using a sectional and a moment method (MOM). Another possibility to solve the PBE is given by Monte Carlo (MC) approaches. Due to their high statistical accuracy, MC models serve as an excellent reference tool for validation purposes. In MC, the particle population is represented by a sufficiently large ensemble of stochastic particles whose size directly influences the computational effort. Thus, a standard MC implementation is not advisable for very detailed models such as investigated here, as the number density of different types of molecules, e.g. stable clusters vs. radical agglomerates, can differ by several orders of magnitude requiring a huge number of stochastic particles. In this study, the soot model of D'Anna and coworkers is implemented in a novel MC framework. Using the concept of scaling, the number of stochastic particles of each molecule type can be chosen independently from the number density of the real system to optimize the computational effort. Application of the model is shown for a fuel-rich, laminar premixed flame.

Steffen Salenbauch
Numerical Thermo-Fluid Dynamics
TU Bergakademie Freiberg
steffen.salenbauch@iec.tu-freiberg.de

Mariano Sirignano, Andrea D'Anna
Universit{a} degli Studi di Napoli Federico II
marianosirignano@yahoo.it, andrea.danna@unina.it

Daniele Marchisio, Marco Vanni
Politecnico di Torino
daniele.marchisio@polito.it, marco.vanni@polito.it

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

CP9

Surrogate Models Based on the Combination of PCA and Kriging

Engineering problems require the use of numerical simulations that require substantial computational resources. Combustion systems fall in this category. They are characterised by very complex physical interactions between chemistry, fluid dynamics and heat transport processes. Usually, a limited amount of resources is available. Thus, the development of reduced-order models is very appealing, both for optimisation as well as for uncertainty quantification, to predict the state of a complex system in a very limited time. Ideally, those reduced models should preserve the physics of the investigated phenomena, and be developed from a limited number of expensive function evaluations, i.e. CFD simulations. The combination of Principal Component Analysys (PCA) with Kriging is considered a promising approach in the attempt to solve this problem. Thanks to PCA, it is possible to enable the extraction of the invariant physics-related information of a combustion-related system and identify the system's coefficients which instead depend on the operating conditions. Kriging is then able to find a response surface for these coefficients. A surrogate model is built that is able to perform parameter exploration with lower computational cost. The combination of the two techniques is the focus of this work. The methodology has already been applied to 1D flames, with a number of input parameters ranging from 1 to 3, and is now demonstrated on more complex systems, i.e. 2D and 3D simulations.

Gianmarco Aversano
Université Libre de Bruxelles
Gianmarco.Aversano@ulb.ac.be

CP9

Improved Extrapolation-Based Stiff ODE Solvers for Combustion CFD

Increasingly large chemical mechanisms are needed to predict autoignition, heat release and pollutant emissions in computational fluid dynamics (CFD) simulations of in-cylinder processes in compression-ignition engines and other applications. Calculation of chemical source terms usually dominates the computational effort, and several strategies have been proposed to reduce the high computational cost associated with realistic chemistry in CFD. Central to most strategies is a stiff ordinary differential equation (ODE) solver to compute the change in composition due to chemical reactions over a computational time step. Most work to date on stiff ODE solvers for computational combustion has focused on backward differential formula (BDF) methods, and has not explicitly considered the implications of how the stiff ODE solver couples with the CFD algorithm. Recently, advantages of extrapolation-based stiff ODE solvers have been demonstrated over BDF methods. In this work, improvements to extrapolation-based solvers with respect to accuracy and speedup are discussed. Further potentials including hydrid (explicit/implicit) integration are demonstrated. Benefits in CPU time and accuracy are shown for homogeneous systems and compression-ignition engines, for chemical mechanisms that range in size from fewer than 50 to more than 7,000 species.

Abdurrahman Imren
The Pennsylvania State University
aui14@psu.edu

Daniel C. Haworth
Pennsylvania State University
dch12@psu.edu

CP9

The Discontinous-Galerkin Method for Chemical Source Term Integration in the Reacting Navier-Stokes Equations

A method for the accurate, fully implicit, integration of chemical source terms for moderately large mechanisms is presented. Using a python library for symbolic mathematics, Sympy, expressions of chemical source terms were re-written as pure analytical functions of species concentrations, gas temperature, and thermodynamic constants. The source term functions were then differentiated with respect to fluid dynamic state variables using Sympy to obtain source term perturbations, source term adjoints, and source term adjoint perturbations. The adjoint and perturbations were added to an existing Discontinuous-Galerkin spacetime finite element code, PROPEL, developed at the

Naval Research Laboratory. The chemical reactions were integrated in time using finite elements of polynomial order one, two, and three to demonstrate high order capabilities. Results show that the chemistry can be integrated along with fluid dynamics at time steps on the order of 1e-3 s. Additionally, the mathematics outlined herein yield grid optimization capabilities, such as adaptivity, and problem optimization capabilities, such as pollutant minimization and reaction sensitivity.

Ryan F. Johnson
Naval Research Laboratory
Laboratory of Computational Physics and Fluid Dynamics
rfjohnson2c@gmail.com

Andrew Corrigan, Douglas Schwer, Andrew Kercher, Kazhikathra Kailasanath
Naval Research Laboratory
andrew.corrigan@nrl.navy.mil, doug.schwer@nrl.navy.mil, andrew.kercher@nrl.navy.mil, kazhikathra.kailasanath@nrl.navy.mil

CP9

Analysis of Operator Splitting Errors for Near-Limit Flame Simulations

High-fidelity simulations of the ignition, extinction and oscillatory combustion processes are of practical interest. Splitting schemes, widely employed in reactive flow simulations, could fail for stiff reaction-diffusion systems exhibiting near-limit flame phenomena. The present work first employs a model perfectly stirred reactor (PSR) problem with an Arrhenius reaction term and a linear mixing term to study the effects of splitting errors on near-limit combustion predictions. Analysis shows that the errors induced by decoupling of reaction and diffusion processes may result in unphysical extinction or ignition. The Strang splitting, the balanced splitting, and a newly developed midpoint method are tested with the prediction of ignition, extinction and oscillatory combustion in unsteady PSRs of various fuel/air mixtures. Results show that the midpoint method can accurately reproduce the dynamics of the near-limit flame phenomena and it is second-order accurate over a wide range of time steps. For the extinction and ignition processes, both the balanced splitting and midpoint method can yield accurate predictions, whereas the Strang splitting can lead to significant shifts on the ignition/extinction processes or even unphysical results. For the sustainable and decaying oscillatory combustion from cool flames, both the Strang splitting and the midpoint method can successfully capture the dynamic behavior, whereas the balanced splitting scheme results in significant errors.

Zhen Lu, Hua Zhou
Center for Combustion Energy, Tsinghua University
luz11@mails.tsinghua.edu.cn, zhouhua12@mails.tsinghua.edu.cn

Shan Li, Zhuyin Ren
Center for Combustion Energy, Tsinghua University
School of Aerospace Engineering, Tsinghua University
lishan14@mails.tsinghua.edu.cn, zhuyinren@tsinghua.edu.cn

Tianfeng Lu
Department of Mechanical Engineering
University of Connecticut
tlu@engr.uconn.edu

Chung K. Law
Dept. Mech. & Aerospace Engr.
Princeton University
cklaw@princeton.edu

CP9

Efficient Numerical Algorithms Using Asymptotic Estimation of Mesh Parameter for Singularly Perturbed Boundary Value Problems with and Without Turning Point

Singular perturbations is a maturing mathematical subject with a long history and continued important applications throughout science and engineering. In this article we would like to present an efficient numerical algorithm for a few classes of singularly perturbed boundary value problems (SPPs) with and without turning point. It is well known that when classical methods on uniform meshes are used to solve SPPs, the result obtained are good only if the input size of the algorithm is very large. Therefore, the classical methods are not appropriate for practical applications if the perturbation parameter is close to some critical value. We would like to present our investigation in the direction of identifying a priori construction of non-uniform mesh based on asymptotic analysis of Shishkin mesh parameter to achieve better accuracy when compared with Shishkin mesh for singularly perturbed problems with and without turning point. The reduction to practice of the proposed algorithm is demonstrated through numerical computations of various SPPs.

Ramesh Vp
Asst. Professor of Mathematics
Central University of Tamil Nadu, India
vpramesh@gmail.com

Prithvi M, Priyanga B
Research Scholar
Central University of Tamil Nadu
moniprithvi14@gmail.com, riyasakar@gmail.com

CP9

Encouraging Modern Software Development Practices for Combustion

Modern combustion research, both computational and experimental, relies on software and computational tools. However, due to a lack of saturation of modern software development practices, researchers often develop their tools in a manner that can take too long, lead to duplicated work, impede reproducibility, and lack verification. This talk will motivate the use of tools and strategies that can save time, ensure trust in computed results, and encourage the adoption, further development, and reuse of research software in combustion and chemical kinetics. Techniques to be introduced include version control, software unit and functional testing, continuous integration, peer code review, reproducibility, benefits of releasing research software openly, and appropriate software citation. These topics will be explored using mature combustion research software such as Cantera and RMG, as well as newer packages like pyJac and PyKED, as examples.

Kyle E. Niemeyer
Oregon State University
Kyle.Niemeyer@oregonstate.edu

Raymond L. Speth
MIT
speth@mit.edu

Bryan W. Weber
University of Connecticut
bryan.weber@uconn.edu

Richard West
Northeastern University
r.west@northeastern.edu

CP10

Premixed Flame Propagation in a Boundary Layer

Methane-air premixed flames propagating in the vicinity of a wall are simulated with complex chemistry and complex transport properties (mixture averaged), using a fourth-order fully compressible flow solver (SiTCom-B). 15 species and 26 reactions are involved in the chemical scheme, which was derived from the GRI-1.2 detailed mechanism, using an automated reduction followed by an optimisation of the rates with a Genetic Algorithm (ORCh method). The wall is either cooled at ambient temperature or heated by the flame, thus solving heat transfer in the solid part of the multi-physics simulations. The chemical structure of the edge-flame propagating near the wall is analysed along with the deviation of the flow streamlines, which is found to control the burning velocity of the propagating front. In additional simulations, the wall is heated by a source upstream of the flame. Depending on the amount of heat added to the system, upstream ignition or enhanced propagation of the initial flame through heat conduction are observed. The controlling mechanisms are analysed in the light of the response of chemistry to the added heat. The complex interaction between the boundary layer and the heat transfer phenomena is further examined comparing the numerical simulations with results from asymptotic developments available in the literature.

Kevin Bioche
CORIA CNRS & INSA ROUEN NORMANDIE
kevin.bioche@insa-rouen.fr

Guillaume Ribert
CORIA - CNRS UMR6614
INSA de Rouen
ribert@coria.fr

Luc Vervisch
INSA Rouen CNRS CORIA
vervisch@coria.fr

CP10

Modeling Radiative Heat Transfer in Gas-Solid Reacting Flows

Radiative heat transfer is an important heat transfer mode in gas-solid reacting flows. Its importance increases recently because of stronger radiation in new combustion technologies, the demand of higher simulation accuracy, and improvements in modeling other processes. Modeling radiative heat transfer requires a spectral model and an Radiative Transfer Equation (RTE) solver in a single-phase flow. The choice of the multiphase model further complicates radiation models. For multiphase flows, an averaging model is usually required. Spectral models could be gray, nongray or a mix of gray and nongray for different phases. Similar to the approach to the dispersed phases, RTE solvers can be Eulerian (e.g., P1 and Discrete Ordinate Methods) or Lagrangian (e.g., Photon Monte Carlo). Because they may be coupled with either an Eulerian or Lagrangian multiphase model, this results in multiple possible model combinations. A generic framework is helpful in bridging the gap between intricate radiation modeling concepts and diverse thermo-chemical environments in applications. This was developed previously for gaseous combustion, and was found flexible, maintainable, usable and extensible. This research extends the previous framework for gaseous combustion to gas-solid reacting flows. Examples from Eulerian and Lagrangian dispersed phases are discussed. Two levels of radiation model comparisons can be made, and provide insights into model choices and new model developments.

Jian Cai
University of Wyoming
University of Wyoming
jcai@uwyo.edu

CP10

Effect of Heat Transfer on Flame Stabilization and Dynamics

Direct numerical simulations using complex chemistry of V-flames stabilized behind cylindrical flame holders are investigated in order to access the impact of heat transfer on the flame response. Three different cases are considered: an adiabatic, an uncooled and a cooled cylinder. For these cases, Flame Transfer Functions are computed and validated against experimental results. The flame responses feature large differences for the three cases and are explained by different flame root dynamics induced by the flame holder temperature. The results highlight the importance of heat transfer to walls for flame stabilization and dynamics.

Abdulla Ghani, Daniel Mejia, Laurent Selle, Thierry Poinsot
IMF Toulouse
ghani@cerfacs.fr, dmejia@imft.fr, laurent.selle@imft.fr, thierry.poinsot@cerfacs.fr

CP10

Heat Release Effects on Turbulence Statistics in Premixed and Nonpremixed Flames

Statistics of turbulent kinetic energy and scalars are obtained from a series of direct numerical simulations of low Mach number spatially-evolving turbulent planar jet flames. In these simulations, hydrogen combustion is modeled using a detailed nine-species chemical kinetic mechanism, and turbulent coflows ensure that high turbulence intensity is maintained through the flame brush. Simulations are performed at the same moderate bulk Reynolds number for both premixed and nonpremixed configurations in addition to an analogous nonreacting configuration (cold flow). Budgets for the transport of turbulent kinetic energy, scalar flux, and scalar variance are obtained conditioned on the progress variable for the premixed flame and on the mixture fraction for the nonpremixed flame and cold flow. These budgets are compared to one another to determine the role of combustion heat release in modifying the dominant terms in these budgets. Two key phenomena will be the focus of the presentation. First, theoretical arguments have been made that the pressure-dilatation term in the turbulent kinetic energy equation is more important

in premixed flames than in nonpremixed flames, and the DNS data will be used to quantify any differences. Second, scalar flux and variance budgets will be compared for reacting and nonreacting scalars in order to determine the direct role of the chemical source term.

Jonathan F. Macart
Department of Mechanical and Aerospace Engineering
Princeton University
jmacart@princeton.edu

Temistocle Grenga, Michael E. Mueller
Princeton University
tgrenga@princeton.edu, muellerm@princeton.edu

CP10

Radiative Heat Transfer Modelling in a Heavy-Duty Diesel Engine

Detailed radiation modelling in piston engines has received relatively little attention to date. Recently, it is being revisited in light of current trends towards higher operating pressures and higher levels of exhaust-gas recirculation, both of which enhance molecular gas radiation. Advanced high-efficiency engines also are expected to function closer to the limits of stable operation, where even small perturbations to the energy balance can have a large influence on system behavior. Here several different spectral radiation property models and radiative transfer equation (RTE) solvers have been implemented in an OpenFOAM-based engine CFD code, and simulations have been performed for a heavy-duty diesel engine. Differences in computed temperature fields, NO and soot levels, and wall heat transfer rates are shown for different combinations of spectral models and RTE solvers. The relative importance of molecular gas radiation versus soot radiation is examined. And the influence of turbulence-radiation interactions is determined by comparing results obtained using local mean values of composition and temperature to compute radiative emission and absorption with those obtained using a particle-based transported probability density function method.

Chandan Paul, Arpan Sircar, Sebastian Ferreyro-Fernandez, Abdurrahman Imren, D. C. Haworth
The Pennsylvania State University
cxp484@psu.edu, azs286@psu.edu, suf157@psu.edu, aui14@psu.edu, dch12@engr.psu.edu

S. Roy
Marquette University
somesh.roy@marquette.edu

W. Ge, M. F. Modest
UC Merced
wge@ucmerced.edu, mmodest@ucmerced.edu

CP10

Turbulence Radiation Coupling in Boundary Layers of Heavy-Duty Diesel Engines

The lack of accurate submodels for in-cylinder radiation and heat transfer has been identified as a key shortcoming in developing truly predictive, physics-based computational fluid dynamics (CFD) models that can be used to develop combustion systems for advanced high-efficiency, low-emissions engines. Recent measurements of wall layers in engines show discrepancies of up to 100% with respect to standard CFD boundary-layer models. And recent analysis of in-cylinder radiation based on the most recent spectral property databases and high-fidelity radiative transfer equation (RTE) solvers has shown that at operating pressures and exhaust-gas recirculation levels typical of modern heavy-duty compression-ignition engines, radiative emission can be as high as 40% of the wall heat losses, that molecular gas radiation (mainly CO2 and H2O) can be more important than soot radiation, and that a significant fraction of the emitted radiation can be reabsorbed before reaching the walls. That is, radiation not only contributes to heat losses, but also changes the in-cylinder temperature distribution, which in turn affects combustion and emissions. The goal of this research is to develop models that explicitly account for the potentially strong coupling between radiative and turbulent boundary layer heat transfer. For example, for optically thick conditions, a simple diffusion model might be formulated in terms of an absorption-coefficient-dependent turbulent Prandtl number.

Arpan Sircar, Chandan Paul, Sebastian Ferreyro-Fernandez, Abdurrahman Imren
The Pennsylvania State University
azs286@psu.edu, cxp484@psu.edu, suf157@psu.edu, aui14@psu.edu

Daniel Haworth
Penn State University
dch12@engr.psu.edu

Somesh P. Roy
Department of Mechanical Engineering
Marquette University
somesh.roy@marquette.edu

Wenjun Ge, Michael Modest
University of California Merced
wge@ucmerced.edu, mmodest@ucmerced.edu

CP11

Large Eddy Simulation of Air-Flow Modulation on the Dynamics of Two-Phase Swirling Flames for Two Different Fuel Injection Technics

Staged multipoint injection has been proposed as a viable option to control unstable phenomena in gas turbines lean premixed prevaporized (LPP) combustors. Nonetheless, thermo-acoustic interactions that are prone to appear for such combustion regimes are still a major concern. The BIMER combustor has been operated for several years to help understand and control the complex processes its usage involves. The burner is composed of two swirling stages: a pilot stage where fuel is injected through a pressurized nozzle and a multipoint stage where fuel is injected through ten equally spaced holes. In the present study, large eddy simulations of the BIMER combustor are carried out with the two-phase flow (TPF) solver AVBP developed by CERFACS and IFPEN. The main objective is to evaluate the impact of thermo-acoustic interactions through two sets of simulations, pilot-only and multipoint-only injection, with and without the introduction of acoustic pulsing. As in the experiments, in the pilot-only case, the flame stabilizes inside the injection system showing a typical V-shape. A strong precessing vortex core and low thermo-acoustic instabilities are observed. In the multipoint-only injection, the flame is totally stabilized in an M-shape inside the combustion chamber with an opposite dynamical behavior. The impact of the modulation of the bulk flow on the flame shape and dynamics is carefully analysed, show-

ing very distinct features.

Leo Cunha Caldeira Mesquita, Artur Carvalho Santos,
Benoit Cheneau
Laboratoire EM2C, CNRS, CentraleSupelec
Université Paris-Saclay
leo.cunha@centralesupelec.fr,
artur.carvalho-santos@student.ecp.fr,
benoit.cheneau@centralesupelec.fr

Aymeric Vié
Laboratoire EM2C
CNRS-CentraleSupélec
aymeric.vie@centralesupelec.fr

Sébastien Ducruix
EM2C Laboratory
sebastien.ducruix@centralesupelec.fr

CP11

Large-Eddy Simulation of Pulverised-Coal Combustion

The ingredients required to perform Large-Eddy Simulation (LES) of pulverized-coal combustion with complex chemistry are discussed. The amount and the composition of the volatiles released by a given coal vary with the heating rate and the temperature applied to the coal particles. The asymptotic case of a high heating rate and high temperature is considered in line with pulverized-coal flames stabilised by a pilot flame. In this context, numerical results obtained with the devolatilization model by Maffei et al. are compared against experiments in a drop tube furnace and a flat flame burner. After estimating the prediction capabilities of this modelling for devolatilization, a 19 species and 28 reactions chemical mechanisms is coupled with the artificially thickened flame model to simulate the swirl-piloted pulverized coal burner studied by Balusamy et al. at Cambridge (UK). A point source Lagrangian approach for the coal particles is coupled in two-way with a low Mach number Eulerian simulation of the carrying flow (YALES2 code), heat transfer by radiation is accounted for in the thermal budget of the coal particles. The mesh is composed of 108M cells with a resolution of the order of 350 micro-meter. A systematic comparisons of the statistical results collected from LES are compared against their experimental counterpart.

Pascale Domingo
CORIA - CNRS UMR6614
pascale.domingo@coria.fr

Dorian Midou
CORIA CNRS & INSA ROUEN NORMANDIE
midou@coria.fr

Luc Vervisch
INSA Rouen CNRS CORIA
vervisch@coria.fr

CP11

A Large Eddy Simulation of a Rotating Detonation Engine

Rotating detonation engines combust reactive gas mixtures with a high-speed, annularly-propagating detonation wave, which provides many advantages over conventional combustors including a stagnation pressure gain and a more compact, lightweight design. However, the non-premixed nature of common fuel-air injection schemes can lead to significant flow-field inhomogeneities, which can affect the character and stability of the rotating detonation wave. Therefore, this work seeks to glean insight into the propagation of the detonation wave using high-fidelity large eddy simulation. A representative six-inch-diameter rotating detonation engine is used for the geometry, and comparisons are made to experimental data. From the simulation, we seek to quantify the effects of mixture stratification and turbulence on the operation of a rotating detonation engine and identify opportunities for design improvement.

Kevin Grogan
Stanford
kgrogan@stanford.edu

Brent Rankin
Air Force Research Laboratory
brent.rankin.1@us.af.mil

John Hoke
Innovative Scientific Solutions Incorporated
john.hoke.4.ctr@us.af.mil

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP11

Large Eddy Simulation and Probability Density Function Modelling of High-Speed Reacting Flows

Scramjet propulsion systems are regarded to be one of the key technologies to deliver the next generation of hypersonic planes. In a scramjet engine combustion occurs at supersonic speeds, this introduce limitations in the degree of mixing and increases the interactions between the chemistry and the flow. Numerical simulations of scramjet combustion shed a light into the physics of supersonic combustion. The present work aims to develop turbulent/combustion numerical models capable to reproduce the physics inside a scramjet. The work formulates a new joint scalar-velocity-energy probability density function (PDF) equation in a Large Eddy Simulation framework. The formulation can deal with compressible reactive flows at low and high Mach numbers. The model reduces the number of unknown correlations in compressible turbulent flow from ten to four. The non-linear reactive terms are treated exactly. The Langevin model and the interaction by exchange with the mean micromixing models are considered to close the remaining unknown terms. In the proposed model, the PDF equation is solved using a Eulerian Stochastic Field. In contrast to Lagrangian-based formulation, the model can be directly implemented in traditional Eulerian-based CFD codes and shows no problem of pressure-velocity coupling. Validation of the model is performed through the simulation of compressible reacting mixing layers. The results are then compared with existing DNS data from the literature.

Yuri Paixao de Almeida
Imperial College London
y.paixao-de-almeida15@imperial.ac.uk

Salvador Navarro-Martinez
Department of Mechanical Engineering
Imperial College

s.navarro@imperial.ac.uk

CP11

Large Eddy Simulation of Reacting Flows at High Pressures Using GPU Acceleration

In high pressure combustors, the dispersion of fuel and the subsequent combustion processes are significantly different from ambient conditions. Simulation of mixing and combustion under such conditions requires a proper treatment of the thermochemical and molecular transport properties including real fluid effects and supercritical phenomena. The combination of complex multi-component property evaluations along with the computational grid resolution requirements makes these simulations expensive and cumbersome. Recent advances in high performance computing (HPC) systems, such as the graphics processing unit (GPU) based architectures provides an opportunity to reduce the time to solution. Here, we present the acceleration of a software for large eddy simulation (LES) of turbulent combustion. A combination of programming models has been used to convert a distributed memory parallel code to a hybrid parallel code with multiple levels of parallelism. Compiler directives are used to add shared memory parallelism for efficient use of multi-core processors. Major performance critical kernels have been re-implemented using a generic programming approach in C++ that allows efficient execution on GPU and other architectures, while ensuring performance portability. Simulation and performance results from the newest GPU accelerated and many-core systems are presented.

Ramanan Sankaran, Kalyana Gottiparthi
Center for Computational Sciences
Oak Ridge National Laboratory
sankaranr@ornl.gov, gottiparthik@ornl.gov

Joseph C. Oefelein
Sandia National Laboratories
Combustion Research Facility
oefelei@sandia.gov

CP12

Concept of Spectral Differentiation for Solving a Flow Model

The concept of differentiation with the first kind of spectral method is used in this presentation to solve the model of movement of flow around an upright angle. In this model, lots of flow features and interactions and separations take a place and hence a high accurate numerical techniques is needed. Because of the singularities in some nodes, we used a conformal mapping which is used by many researchers. A numerical simulation of the fluid movements will be showed along side with some tables to validate our results with others.

Badr Alkahtani
King Saud University
alhaghog@gmail.com

CP12

Dissipation Element Analysis of Premixed Spatial Evolving Jet Flames

Dissipation element analysis is a tried and tested method to analyze scalar fields in turbulent flows. Dissipation elements are defined as an ensemble of grid point whose gradient trajectories reach the same extremal points. Therefore, the scalar field can be compartmentalized in monotonous space filling regions. Dissipation elements can be statistically described by two parameters, namely the Euclidean distance between their extremal points and their scalar difference in these points. The joint probability density function of these two parameters is expected to suffice for a statistical reconstruction of the scalar field. In addition, normalized dissipation element statistics show an invariance towards changes in Reynolds numbers. The dissipation element analysis is applied to a set of spatial evolving premixed jet flames at different Reynolds number. The simulations feature finite rate chemistry with 16 species and 73 reactions and up to 22 Billion grid points. The jet consists of a methane/air mixture with equivalence ratio $\phi = 0.7$ and temperature T=800K. The temperature and species concentrations in the coflow correspond to the equilibrium state of the burnt mixture. All the simulations are performed at 4 atm. Marginal and joint statistics of dissipation element parameters are shown and compared to those of a DNS of a non-reacting spatial jet and isotropic turbulence. In addition, correlation between chemical species and dissipation elements is investigated.

Dominik Denker
RWTH Aachen University
Institut für Technische Verbrennung Aachen Univerity
ddenker@itv.rwth-aachen.de

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Stefano Luca
King Abdullah University of Science and Technology
stefano.luca@kaust.edu.sa

Fabrizio Bisetti
University of Texas at Austin, USA
fbisetti@utexas.edu

Heinz Pitsch
Aachen University
h.pitsch@itv.rwth-aachen.de

CP12

A Variational Approach to Design a Numerical Scheme on an Arbitrary Moving Grid for N-Fluid Flow with Thermodynamic Consistency

In some highly demanding fluid dynamics simulations, ranging from chemical combustion to inertial confinement fusion, it appears necessary to simulate multi-fluid flows involving numerous constraints at the same time, such as (and non-limitatively): large numbers of fluids (typically 10 and above), both isentropic and strongly shocked compressible evolutions, large heat sources, large deformations, transport over large distances, and highly variable or contrasted EOS stiffness. Fulfilling such a challenge in a robust and tractable way demands that thermodynamic consistency of the numerical scheme be carefully ensured. This is addressed here over an arbitrarily evolving computational grid (Arbitrary Lagrange–Euler) by a three-step mimicking derivation: i) For compatible (approximately symplectic) exchange between internal and kinetic energies under isentropic conditions, a least action principle is used to generate the proper pressure forces in the momentum equations; ii) For energy conservation, a tally is performed to match the internal and kinetic energies, and iii) For shock capture,

artificial dissipation is added (other physical terms could also be included such as drag, heat exchange, etc.). Varied single-, two- and multi-fluid test cases show satisfactory behavior, including the 2D supersonic, high volume-fraction convergence of eight Gaussian packets of different fluids in a background of perfect gas (under the sole pressure coupling).

Antoine Llor
CEA
antoine.llor@cea.fr

Thibaud Vazquez-Gonzalez
CEA Bruyeres le Chatel
thibaud.vazquez-gonzalez@cea.fr

Christophe Fochesato
CEA
christophe.fochesato@cea.fr

CP12

On the Suitability of Deconvolution to Capture Filtered Premixed Flames Structure and Propagation

A possible modeling approach in LES of reactive flows is to deconvolve resolved scalars. By inverting the LES filter, scalars such as mass fractions are reconstructed. This information can be used to close budget terms of filtered species balance equations, such as the filtered reaction rate. Being ill-posed in the mathematical sense, the problem is very sensitive to any numerical perturbation. The objective of the present study is to assess the ability of this kind of methodology to capture the chemical structure of premixed flames. For that purpose, four deconvolution methods are tested on a 1-D filtered laminar premixed flame configuration: the Approximated Deconvolution Method (ADM) based on Van Cittert iterative deconvolution, a Taylor decomposition-based method, the Regularized Deconvolution Method (RDM) based on the minimization of a quadratic criterion and finally a new method coupling ADM with a subgrid scale profile reconstruction using parametric functions. Conducted tests analyze the ability of the method to capture the chemical filtered flame structure and front propagation speed. Results show that the deconvolution model should include information about small scales in order to regularize the filter inversion. A priori and a posteriori tests showed that the filtered flame propagation speed can then be well captured if the filter size is not too large.

Cedric C. Mehl
EM2C laboratory, CentraleSupelec
cedric.mehl@centralesupelec.fr

Jerome Idier
IRCCyN laboratory
jerome.idier@irccyn.ec-nantes.fr

Benoit Fiorina
Laboratoire EM2C, Ecole Centrale Paris
benoit.fiorina@centralesupelec.fr

CP12

Architecture-Aware Dynamic Repartitioning for Turbulent Reactors

Hybrid Eulerian-Lagrangian flow solvers are commonly used for the simulation of turbulent reacting flows. Due to turbulence-chemistry interactions these simulations are typically very costly. Moreover, the evolving regions of chemical reaction present unique challenges for designing efficient parallel solvers. The concepts of load balancing, (re)partitioning, and data migration become important design considerations. We have developed PARAGON, an architecture-aware graph repartitioner, to address these challenges. PARAGON considers the performance impact of nonuniform network communication costs and contention on the memory subsystems of modern multicore clusters. We compare the performance of this new tool to Zoltan, developed at Sandia National Laboratories, which provides parallel partitioning, load balancing and data-management services. A scalability analysis and performance assessment is conducted for the case of a hybrid Eulerian-Lagrangian flow solver with reduced order, finite-rate kinetics as applied to a Taylor Green vortex flow with chemical reaction.

Peyman Givi
University of Pittsburgh, USA
Givi@engr.pitt.edu

Patrick Pisciuneri
University of Pittsburgh
php8@pitt.edu

CP12

Adaptive Numerical Solution of Advancing and Retreating Edge Flames in a New Configuration

We study canonical edge flames to model extinction, reignition, and flame lifting in turbulent non-premixed combustion. An adaptive-resolution finite-element method is used to solve for laminar edge flames in the moving frame of reference with respect to a spatially developing mixing layer. We solve the variable-density zero Mach number Navier-Stokes equations using a homotopy method. The propagation speed of the edge flame is determined simultaneously (implicitly) with the scalar fields both for advancing and retreating flames. Pseudo arc-length continuation is used for parametric tracing of the propagation speed as a function of reaction rate strength. Edge flame behavior as a function of strain and Lewis numbers will be discussed.

Ben Shields
University of Illinois at Urbana-Champaign
bshield2@illinois.edu

Carlos Pantano
Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
cpantano@illinois.edu

Jonathan B. Freund
University of Illinois at Urbana-Champaign
jbfreund@illinois.edu

CP13

Virtual Chemistry Applied to Pollutants Emission Prediction

Chemical flame structures encountered in practical combustors are complex because multiple regimes coexist. Combustion modeling strategies based on single flame archetype fail to predict pollutant species, especially CO. To account for mixed combustion regimes at a reduced computational cost a novel approach based on virtual optimized mechanisms has been recently proposed. This

method consists in i) building a kinetic scheme from scratch instead of reducing a detailed mechanism and ii) using virtual reactions and virtual species that do not represent real entities. In the present work, kinetic rate parameters and virtual species properties are optimized through a genetic algorithm to properly capture the flame/flow field interaction and CO emissions for both premixed and non-premixed flame archetypes. The proposed virtual scheme is first evaluated on laminar flames showing a good agreement for the two targeted flame properties. Then a DNS simulation of a 2-D laminar tribrachial flame is performed to challenge the developed virtual kinetic scheme on a configuration featuring different combustion regimes. The performances of the virtual model in terms of prediction and computational cost are compared against detailed chemistry, analytically reduced chemistry and a global mechanism.

Mélody Cailler
Laboratoire EM2C CNRS, CentraleSupélec
Safran Tech
melody.cailler@centralesupelec.fr

Nasser Darabiha
Laboratoire EM2C
CNRS-CentraleSupélec
nasser.darabiha@centralesupelec.fr

Denis Veynante
Laboratoire EM2C CNRS, CentraleSupélec
denis.veynante@centralesupelec.fr

Benoit Fiorina
Laboratoire EM2C, Ecole Centrale Paris
benoit.fiorina@centralesupelec.fr

CP13

Adjoint-Based Sensitivity of Ignition in Non-Premixed Turbulent Flows

The uncertainty of ignition success in non-premixed turbulent flows remains a fundamental challenge in many practical combustion systems. Mapping the spatial distribution of ignition probability often relies on trial-and-error testing, which becomes prohibitive when measuring sensitivity to a large number of parameters or varied flow conditions. An alternative approach is to formulate the adjoint of the perturbed and linearized governing equations in such a way that sensitivity of ignition to an arbitrarily large number of parameters can be obtained simultaneously via its solution. Our previous studies have shown that it is possible to obtain precision-limited sensitivity gradients for high-fidelity schemes which are attractive for simulating turbulent combustion. However, it remains unclear in general how well local sensitivity can describe nonlinear and unsteady processes. Moreover, adjoint methods are known to suffer from cumulative error growth that results from chaos, which is expected to be significant in turbulent combustion. In this study we perform direct simulations of a non-premixed turbulent shear layer and compute the corresponding discrete-exact adjoint to obtain sensitivity of ignition to a set of design parameters. Different quantities of interest that quantify ignition success are considered, and the impact of this choice on sensitivity is addressed. The influence of flow realization and ignition source placement on sensitivity calculations is also reported.

Jesse Capecelatro
University of Michigan
jcaps@umich.edu

Jonathan B. Freund
University of Illinois at Urbana-Champaign
jbfreund@illinois.edu

CP13

Impact of Chemical Kinetic Model Reduction on Premixed Multi-Dimensional Flame Characteristics

The use of detailed chemical kinetic models for direct numerical simulations (DNS) is prohibitively expensive. Current best practice for the development of reduced models is to match homogeneous ignition delay times and laminar burning parameters such as flame speed and thickness to predictions from the detailed chemical kinetic models using zero- or one-dimensional calculations. Prior studies using reduced models implicitly assume that matching the homogeneous and laminar properties of the detailed model in a single-dimensional case will result in similar behavior in multi-dimensional laminar and turbulent simulations. However, this assumption has not been tested. Fillo et al. recently demonstrated experimentally that real jet fuels with similar chemistry and laminar burning parameters exhibit different sensitivities to multi-dimensional effects such as flame stretch. This result raises questions about the validity of current best practices for the development of reduced chemical kinetic models for turbulent DNS. This study will investigate the validity of current best practices. Combustion parameters, including flame speed, thickness, and stretch rate, will be compared for three skeletal models for the Princeton POSF 4658 surrogate model, reduced using current best practice methods. DNS calculations of premixed, multi-dimensional flames will be compared to determine if these methods are valid.

Aaron J. Fillo
Oregon State University
School of Mechanical, Industrial, and Manufacturing Eng.
filloa@oregonstate.edu

Kyle E. Niemeyer
Oregon State University
Kyle.Niemeyer@oregonstate.edu

CP13

Effect of Mechanism Reduction on the Uncertainty Quantification of Chemical Kinetics for MILD Combustion

In Moderate or Intense Low-oxygen Dilution (MILD) combustion the mixing time scale and the chemical time scale are in the same order of magnitude. This implies that a detailed chemical mechanism should be used to accurately represent these conditions through computer simulations. However, existing detailed chemical mechanisms have been optimized and validated for conventional combustion, and the performance for MILD combustion is inadequate. To improve the proficiency of chemical mechanisms during these conditions, Uncertainty Quantification (UQ) can be used to quantify and minimize uncertainties in the chemical mechanism with respect to MILD combustion targets. While the use of detailed chemical mechanisms is essential for MILD combustion, some species and reactions may not be relevant in these conditions. Mechanism reduction schemes can therefore be applied in order to reduce the computational time, while still preserving accuracy of the simulations. Depending on which species and reactions

that are removed from the mechanism, there could be an effect on the UQ process which should be considered. Coupling UQ with mechanism reduction for MILD combustion is therefore the focus of this work.

Magnus Fürst
Université Libre de Bruxelles
magnus.furst@ulb.ac.be

Alessio Frassoldati
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
alessio.frassoldati@polimi.it

Alessandro Parente
Université Libre de Bruxelles
alessandro.parente@ulb.ac.be

CP13

A Reduced Chemical Mechanism for Kerosene via an RCCE-CSP Methodology

A detailed mechanism for the oxidation of kerosene may contain hundreds of species and thousands of reactions, postulating the use of reduced chemical mechanisms. Rate-Controlled Constrained Equilibrium (RCCE) is a systematic method for the reduction of mechanisms, according to which the slow species are evaluated from the chemical kinetics of the detailed mechanism, while the fast species are assumed to be in an equilibrium state that is constrained by the slow species, through a minimisation of an energy function. The selection of these species relies on the separation of time-scales, which is here investigated with Computational Singular Perturbation (CSP). The reduced mechanism is derived from one-dimensional non-premixed flamelets with varying strain rate, and consists of 42 species out of 369 species in the detailed mechanism with a surrogate fuel based on n-dodecane. Subsequently, the mechanism is not only tested successfully in non-premixed flamelets, but also in one-dimensional premixed flames, perfectly stirred reactors and in flamelets with time-dependent strain rate to evaluate the dynamics of the reduced mechanism. An overall very good agreement is obtained in all problems, indicating that the mechanism can be employed in a wide range of combustion regimes, not restricted to the ones employed for its derivation.

Panayiotis Koniavitis, W. P. Jones
Imperial College London
p.koniavitis13@imperial.ac.uk, w.jones@imperial.ac.uk

Stelios Rigopoulos
Imperial College London
Department of Mechanical Engineering
s.rigopoulos@imperial.ac.uk

CP13

Rapid Reduction of a Chemical Kinetic Model for the Combustion of the Pyrolysis Oil Surrogate Ethylene Glycol

This work focusses on the reduction of a chemical kinetic mechanism based on a novel linear transformation model which is numerically inexpensive. As an example, the method is applied to a newly developed detailed chemical kinetic model for the combustion of ethylene glycol—a substance being used as a surrogate for pyrolysis oil. In the first step of the rapid reduction, this model is reduced for atmospheric combustion conditions in air. Thereby, the extent of the chemical kinetic model is significantly reduced from 85 to 29 species, including the inert species N_2 and Ar, and reduced from 643 to 132 reactions. In the second step of the rapid reduction, the reduced model is subsequently optimized with target data, species profiles from homogeneous combustion and laminar flame speeds, which are created numerically with the detailed model. With this subsequent optimization the reduced model is capable to numerically recreate this target data with high accuracy for a wide range of conditions. The numerical effort of this complete reduction procedure is low and the procedure is highly automatable. The computational time of this procedure takes around half an hour on 32 state of the art CPUs.

Torsten Methling
German Aerospace Center (DLR)
Institute of Combustion Technology
torsten.methling@dlr.de

Trupti Kathrotia
German Aerospace Center (DLR), Institute of Combustion
Technology
trupti.kathrotia@dlr.de

Uwe Riedel
German Aerospace Center
uwe.riedel@dlr.de

CP14

LES Investigation of Fuel Effects on Lean Blow off (LBO) for a Realistic Two-Phase Flow Combustor

The development of gas turbines that operate at lean conditions is needed to meet increasingly stringent emission regulations. By operating at lean conditions lower temperatures are observed in the combustor chamber and a reduction of NOx emissions is achieved. However, in lean conditions these gas turbines are susceptible to blowout as the flame stabilization mechanisms are weakened. In the present work, the lean blow-out (LBO) limit is investigated in order to observe the combustion dynamics near blowout and determine optimal operating conditions. This is accomplished using large-eddy simulations of a realistic two-phase flow combustor operating near the LBO limit. Liquid spray is modelled using a polydisperse droplet injection with stochastic modeling of droplet breakup and a Lagrangian spray evaporation model. The flow field and gas phase chemistry is solved using an unstructured Navier-Stokes solver for complex geometries and a flamelet/progress variable formulation, respectively. The effect of fuel composition is investigated to determine its impact on the LBO limit and the transition from stable operating conditions to blowoff.

Jeffrey Labahn, Lucas Esclapez
Stanford University
jwllabah@stanford.edu, lesclape@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP14

Large Eddy Simulation of Non-Conventional Com-

bustion Regimes

During the past few decades, a number of innovative combustion technologies has been proposed. One of the most promising technologies, Moderate or Intense Low-oxygen Dilution (MILD) combustion, features very low NOx and CO emission, while ensuring very high efficiency. The present work focuses on the validation of numerical simulation of turbulent combustion under MILD conditions, in the Adelaide Jet-in-Hot-Coflow (JHC) burner. The Adelaide JHC burner has a central jet with methane and hydrogen on the molar basis of 50/50. A hot co-flow with diluted oxygen is provided in the annulus region to ignite the central jet fuel. Experimental data of species mass fraction and temperature are available for comparison. Closures based on the Perfectly Stirred Reactor (PSR) and Partially Stirred Reactor (PaSR) concepts are selected as sub-grid models for the finite rate chemistry. The pimple algorithm is implemented in the transient solver. Stiff chemistry is handled with the OpenSMOKE library. Currently, the RANS simulation of the JHC burner has been conducted showing the sensitivity of the results to different modeling parameters and numerical approaches. Based on the results, Large Eddy Simulation are being performed with global chemistry, to adjust the inflow boundary conditions. Then, LES of the JHC case will be extended to include detailed chemistry.

Zhiyi Li
Aero-Thermo-Mechanics Department
Université libre de Bruxelles
zhiyi.li1990@gmail.com

Alberto Cuoci
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
alberto.cuoci@polimi.it

Amsini Sadiki
Department of Energy and Power Plant Technology,TU Darmstadt
sadiki@ekt.tu-darmstadt.de

Alessandro Parente
Université Libre de Bruxelles
alparent@ulb.ac.be

CP14

Large Eddy Simulation of Lifted Turbulent Flame Using Doubly Conditional Source-Term Estimation

Lifted turbulent flames are found when the fuel injection or coflow velocity is too high for stabilization at the burner rim. In atmospheric cold air, without autoignition, these flames stabilize in a partially-premixed combustion mode. The present study is focused on simulating a series of lifted turbulent jet flames stabilized in cold air at different Reynolds numbers using Large Eddy Simulation (LES) coupled with Doubly Conditional Source-term Estimation (DCSE) to reproduce the partially-premixed flame stabilization mechanism. Detailed chemistry is incorporated using Trajectory-Generated Low Dimensional Manifolds (TGLDM). The objectives of the present work are to implement a reliable LES-DCSE methodology to simulate lifted turbulent flames and assess the current models to predict the lift-off height. As a first step, one Reynolds number will be considered. The numerical predictions that will be presented include methane concentrations at different locations throughout the flame and the lift-off height. The numerical results will be compared with previous values obtained by Reynolds-Averaged Navier Stokes (RANS) calculations and available experimental data.

Mohammad Mortada, Cecile B. Devaud
University of Waterloo
Mechanical and Mechatronics Engineering
m7mostaf@uwaterloo.ca, cdevaud@uwaterloo.ca

CP14

LES of Core Noise in a Combustor Nozzle System

As the noise generated by other acoustic sources is reduced, combustion or core noise has emerged as a growing concern for aero-engine designers. This work centers on numerical simulation of an experiment of a dual-swirl methane-air combustion chamber with the exhaust passing through a transonic converging-diverging nozzle performed at DLR Berlin (Bake et al., 2009). Large Eddy Simulation (LES) is used to predict the in-chamber and downstream acoustics, and these pressure spectra, as well as velocity and flame structure predictions, are validated against DLR's experimental results. Modal decomposition is applied to the fields inside the combustion chamber to provide additional insight into the dynamics leading to sound production. The focus of the downstream portion of the domain is on probing the sensitivities of indirect noise mechanisms, including the recently discovered composition noise mechanism (Ihme, 2017; Magri et al., 2016) which predicts that fluctuations in mixture fraction can give rise to indirect noise. This work represents the first three dimensional, high-fidelity evidence of the low order composition noise theory. Other aspects of indirect noise generation, including sensitivity to non-planar waves and fluctuation spatial structure, are examined in detail as well. All results, including composition effects, are compared against existing low order theory.

Jeffrey D. O'Brien
Stanford University - Center for Turbulence Research
jobrien@stanford.edu

Friedrich Bake
German Aerospace Center
friedrich.bake@dlr.de

Yu Lv
Stanford University
ylv@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP14

Large Eddy Simulation of Co2 Dilution in Premixed Swirling Oxy-Flames and Assessment of Radiation Effects

The very high temperature of burnt products in oxy-combustion burners is usually tempered with the recirculation of exhaust gases, such as CO_2. The effect of this dilution on the flame stabilization has been investigated experimentally in comparison to conventional methane-air flames. Two configurations (CH_4/air and $CH_4/O_2/CO_2$ flames) have been retained for the present numerical study. The challenge is to retrieve both flames behavior with the

same modeling approach. The validation is carried out by comparing with experimental fields of velocity, OH^* chemiluminescence and burnt gases probability distribution deduced from OH-PLIF. For both configurations, large-eddy simulations (LES) are performed with the F-TACLES (Filtered Tabulated Chemistry for LES) combustion model which is based on tabulated chemistry to account for complex chemistry at low computational cost in premixed flames. After an initial simulation under adiabatic wall conditions, wall heat losses are accounted for by i) imposing the measured wall temperature in the LES and ii) accounting for the enthalpy defect in the tabulated chemistry model. Finally, given the high concentration of CO_2, radiation effects are very likely to be significant. To account for radiation emission and absorption in the burnt gases, a reciprocal Monte-Carlo method is used to accurately assess the importance of radiation in the different configurations.

Lorella Palluotto
EM2C laboratory
lorella.palluotto@ecp.fr

Ronan Vicquelin
EM2C, CNRS, Ecole Centrale Paris
ronan.vicquelin@centralesupelec.fr

Paul Jourdaine, Clément Mirat, Thierry Schuller
EM2C laboratory
paul.jourdaine@ecp.fr, clement.mirat@ecp.fr,
thierry.schuller@ecp.fr

Olivier Gicquel
EM2C Laboratory
Ecole Centrale Paris
olivier.gicquel@ecp.fr

CP14

LES-FDF with Hybrid Finite Rate and Flamelet Chemistry Modeling of a Piloted Turbulent Flame with Inhomogeneous Inlets

A hybrid large eddy simulation (LES) method combining flamelet tabulation with transported filtered density function (FDF) finite rate chemistry strategies has been developed and applied to simulate the Sydney/Sandia piloted turbulent flame with inhomogeneous inlets [Meares & Masri, 2014; Barlow et al., 2015]. The flame is reported to exhibit stratified-premixed as well as diffusion-dominated modes, which renders classical combustion models that either work for premixed or non-premixed flames intractable to accurately predict this flame. The method presented combines the combustion regime independent transported FDF method with a computationally cheap flamelet-based method in a hybrid manner. The computationally expensive Lagrangian particles representing the transport of the FDF are seeded only in certain locations whereas the rest of the domain is treated with flamelet chemistry based on the LES transported fields and an appropriate presumed PDF closure. The method relies on consistency between Eulerian and Lagrangian fields through robust coupling. Seeding of the particles is based on LES transported mixture fraction, its variance and a progress variable. The performance of the hybrid model is verified by an extensive comparison to the experiment including mean and rms profiles of species, conditional averages and scatter plots. It is also shown that the method can efficiently be used for flames exhibiting local extinction and finite rate chemistry effects.

Martin Rieth
University of Duisburg-Essen
martin.rieth@uni-due.de

Suresh Menon
Georgia Inst. of Technology
Sch.of Aerospace Engineering
suresh.menon@aerospace.gatech.edu

Fabian Proch
Chair of Fluid Dynamics
University of Duisburg-Essen
fabian.proch@uni-due.de

Andreas Kempf
Duisburg-Essen University
andreas.kempf@uni-due.de

CP15

Dynamic Mode Decomposition of Turbulent Non-Reacting and Reacting Nonpremixed Jets

Dynamic Mode Decomposition (DMD) decomposes data into coherent modes with corresponding growth rates and oscillatory frequencies, allowing for the investigation of unsteady and dynamic phenomena unlike conventional statistical analyses. The method identifies structures unbiased by energy so is particularly well suited to exploring dynamic processes at scales smaller than the largest, energy-containing scales of the flow. In this work, DMD is used as a tool to analyze a series of large three-dimensional Direct Numerical Simulations of low Mach number spatially-evolving turbulent planar nonpremixed hydrogen/air jets both reacting and non-reacting. The focus of this investigation will be on the physical insights that may be derived from the DMD modes and changes in the modes associated with combustion heat release.

Temistocle Grenga
Princeton University
tgrenga@princeton.edu

Jonathan F. Macart
Department of Mechanical and Aerospace Engineering
Princeton University
jmacart@princeton.edu

Michael E. Mueller
Princeton University
muellerm@princeton.edu

CP15

No_x Formation in Turbulent Premixed Slot Flames with Mixture Inhomogeneity: A Numerical Study

A set of Direct Numerical Simulations of three-dimensional methane/air lean flames in a spatially developing turbulent slot burner are performed. The flames are in the thin-reaction zone regimes and the jet Reynolds number is 5600. This configuration is of interest since it displays turbulent production by mean shear as in real devices. The gas phase hydrodynamics are modeled with the reactive, unsteady Navier-Stokes equations in the low Mach number limit. Combustion is treated with finite-rate chemistry. The jet slot width is H=1.2 mm and the computational domain is 24Hx16Hx4H discretized with 1440x920x256 points

for a total of 350 Million cells. The jet is characterized by a non-uniform equivalence ratio at the inlet and varying levels of incomplete premixing for the methane/air mixture are considered. The global equivalence ratio is 0.7 and temperature is 800 K. All simulations are performed at 4 atm. The instantaneous profiles of the mass fractions of methane and air at the inlet are sampled from a set of turbulent channel simulations that provide realistic, fully turbulent fields. The data are analyzed to study the influence of partial premixing on the flame structure. Particular focus is devoted to the assessment of heat release rate fluctuations and NO_x formation. In particular, the effects of partial premixing on the production rates for the various pathways to NO_x formation are investigated.

Stefano Luca
King Abdullah University of Science and Technology
stefano.luca@kaust.edu.sa

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Fabrizio Bisetti
University of Texas at Austin, USA
fbisetti@utexas.edu

CP15

Generalized Turbulent Combustion Model for Multi-Modal Combustion

Roughly speaking, turbulent combustion models can be divided into two broad classes: models that make no assumption about the underlying combustion processes and models that constrain the underlying combustion processes to some a priori presumed low-dimensional manifold. The former class of models, including Transported PDF (TPDF) and Linear Eddy Model (LEM), is by nature more general but comes at increased computational cost. The latter class of models, including 'flamelet' and 'flamelet'-like models such as Conditional Moment Closure (CMC), is computationally more efficient albeit with the need to assume something a priori. In this work, a new turbulent combustion model for LES is presented that breaks this trade-off, essentially a generalization of 'flamelet' models that requires no a priori assumption about the underlying combustion processes. The model is constructed by first assuming that all (adiabatic, isobaric, two-stream) combustion processes can be described on two-dimensional manifold consisting of a mixture fraction and a generalized progress variable on the unity square. A transformation of the governing equations is performed into these coordinates to describe the evolution of the manifold, and this also provides an explicit definition for the generalized progress variable. This two-dimensional space is shown to recover the three asymptotic modes of combustion under certain limits. Extensions of the model to consider additional physics will also be discussed.

Michael E. Mueller
Princeton University
muellerm@princeton.edu

CP15

Turbulent Flame Sub-Grid Scale Modeling with High-Order Spectral Difference

A novel approach to Large-Eddy Simulation (LES) of turbulent combustion is discussed in the context of high-order Spectral Difference (SD). In these numerical methods, the scalar signals and their corresponding fluxes are approximated through polynomial expansions. It is proposed to extend this polynomial decomposition to the chemical sources of chemical species. A sensor constructed from the modal decay rate of the polynomial approximation of the chemical source allows for automatically locating flow zones where the mesh resolution is too coarse for the flame signal (i.e. source terms) to be resolved. This sensor is easily related to a thickening factor in order to calibrate, from a direct treatment of the scalar signal seen in the simulation, an artificially thickened flame closure. A similar treatment is applied to the components of the scalar gradients, to calibrate the sub-grid scale flame wrinkling factor from the energy of the modes of the resolved scalar gradient. The method is first applied to one-dimensional flames at various mesh resolutions and orders of discretisation. In a second part, a three-dimensional reactive mixing layer is simulated. Starting at a high level of resolution, the mesh is made coarser and statistical results of the various simulations are compared.

Luc Vervisch
INSA Rouen CNRS CORIA
vervisch@coria.fr

Eurielle Bossennec, Guido Lodato
CORIA CNRS & INSA ROUEN NORMANDIE
bossenne@coria.fr, lodato@coria.fr

CP15

Large Eddy Simulation of a Turbulent Swirling Premixed Flame Coupling the TFLES Model with a Dynamic Wrinkling Formulation

Dynamic models that take advantage of the known resolved scales to automatically adjust the model parameters have proved to be very effective in large eddy simulations (LES). Global (uniform parameter evolving only with time) and local (parameter evolving both in space and time) dynamic formulations for the flame wrinkling factor are combined with the Thickened Flame (TFLES) model and simulations of the semi-industrial PRECCINSTA burner studied experimentally by Meier et al. (2007) are performed for the stable and unstable configurations. For the stable flame, dynamic and non-dynamic approaches capture flow and combustion statistics, both in terms of Favre and quasi-Reynolds averages, with good accuracy. Interestingly, the self-excited mode is reproduced only when the dynamic formalism is employed. A mesh convergence proves that the observed instability is not the result of a numerical artifact and a different mechanism other than the hypothesis of imperfect mixing, as suggested by Franzelli et al. (2012), can influence the flame pulsation. Dynamic models may then play an important role in the prediction of combustion instabilities.

Pedro S. Volpiani
Laboratoire EM2C
CNRS, CentraleSupelec, Université Paris-Saclay
pedro.stefanin-volpiani@ecp.fr

Thomas Schmitt
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr

Denis Veynante
EM2C Laboratory
Ecole Centrale Paris

denis.veynante@ecp.fr

CP15

Transitional Behavior in the Regime from Lifted Flames to Mild Flames

Turbulent lifted flames in hot and diluted environments attracted numerous study since its wide application. Autoignition was proven a key factor in stabilizing these flames[1]. When lowering coflow temperature and oxygen ratio towards MILD conditions, namely a transitional flame is found with an extending distribution of CH_2O to jet exit and OH transition from weak to strong at liftoff height, suggesting enhanced preignition[2]. The current study uses LES/FPV approach to simulate behavior and structure of transitional flame. Two coflow conditions at different temperatures with same composition are considered, corresponding with lifted flames and transitional ones. Temporal-spatial-resolved ignition processes are revealed in both cases. Faint triple flame structure is found at flame base, indicates partial premixing stabilizing both flames, however denser CH_2O distribution shown in the transitional flame indicates stronger partial premixing. A moderate reaction zone in lifted region suggests potential existence of MILD regime at the very transition state. Statistical results confirm difference of CH_2O distribution between cases, besides, conditional statistics on mixture fraction showed diverse reaction paths of CH_2O under these conditions.

Chengyu Liu, Jian Zhang
Institute of Mechanics, Chinese Academy of Science
liuchengyu@imech.ac.cn, zhangjian@lnm.imech.ac.cn

Yanhong Ma
School of Energy and Power Engineering
Beihang University
mayanh2002@163.com

CP16

Bayesian Analysis of Constrained Equilibrium Reduced Kinetics Model Parameterization

Bayesian inference is used to quantify parametric and predictive uncertainties associated with the choice of represented species in rate-controlled constrained equilibrium (RCCE) reduced models. Shock-tube experimental measurements of hydrogen-air ignition delay times are used to inform the candidate model classes, which are then ranked quantitatively based on closeness of fit as it is balanced within the model selection framework via penalization of parametric complexity. It is found that as model size increases the best representations given the data form a chain with root H_2-O_2-H. Therefore, they can be successively constructed by adding the species that maximize the likelihood to this root. Finally, predicted ignition delay times issued by the ranked model classes are compared to those obtained using detailed mechanisms. It is shown that, while some detailed mechanisms fail to reproduce the experimental data, RCCE reduction alleviates this mismatch.

Esteban Cisneros-Garibay
University of Illinois at Urbana-Champaign
csnrsgr2@illinois.edu

Carlos Pantano
Mechanical Science and Engineering
University of Illinois at Urbana-Champaign
cpantano@illinois.edu

Jonathan B. Freund
University of Illinois at Urbana-Champaign
jbfreund@illinois.edu

CP16

pyMARS: A open software package for chemical kinetics model reduction

Chemical kinetic models play a crucial role in the simulation of combustion. They provide a model of the chemical reactions present, and the species contained in those reactions. Detailed mechanisms can contain hundreds to thousands of independent species, and thousands to tens of thousands of reactions. Because the computational cost to perform simulations using these models can become impractical, model reduction plays an active part in enabling future research. This presentation will introduce pyMARS (Python-based Model Automated Reduction Software), an open-source software package that performs model reduction using a variety of methods, using the Cantera suite to handle chemical kinetics. These include the directed relation graph (DRG), DRG with error propagation (DRGEP), DRG-aided sensitivity analysis (DRGASA), and DRGEP with sensitivity analysis (DRGEPSA) methods. pyMARS currently generates thermochemical data for reduction and evaluates the error of potential skeletal models using autoignition simulations. Future versions of pyMARS will include additional skeletal reduction methods, and serve both as a tool for reduction of large kinetic models and a testbed for determining optimal reduction strategies.

Parker Clayton, Kyle E. Niemeyer
Oregon State University
claytonp@oregonstate.edu,
Kyle.Niemeyer@oregonstate.edu

CP16

Propagation of Kinetic Uncertainty Through Surrogate Subspace in Turbulent Combustion Simulations

In combustion simulations with uncertainty quantification, the uncertainties of elemental reactions are in general treated independent so that a large number of samples from the high-dimensional uncertainty parameter space are needed to propagate the kinetic uncertainty to global combustion characteristics such as the ignition delay time. It is computationally challenging to perform so many individual turbulent combustion simulations. In this study, a novel approach is proposed to propagate kinetic uncertainty through constructing a one-dimensional surrogate subspace in the parameter space to reproduce the uncertainty on the target quantity. Specifically, the surrogate subspace is constructed by imposing correlations among the uncertainties of the elemental reactions, and the uncertainty factor of each reaction rate is tuned to reproduce the uncertainty of the target quantity using a genetic algorithm. We first demonstrate the construction of the surrogate subspace for hydrogen/air autoignition processes with a 33-reactions detailed mechanism, in which artificial neural network is employed to construct the surrogate model to propagate the uncertainties in reaction rates to the uncertainties on the ignition delay time. Then the mean and variance of the ignition delay time are specified as objective

[1] R.L. Gordon, A.R. Masri, E. Mastorakos, *Combust. Flame*, 155, 181–195.

[2] P.R. Medwell, P.A.M. Kalt, B.B. Dally, *Combust. Flame*, 152, 100–113.

functions for the optimization. Finally the constructed surrogate subspace is applied to propagate the kinetic uncertainty in the transported PDF simulations of Cabra flame.

Weiqi Ji
Tsinghua University
jiweiqi10@163.com

Jiaxing Wang, Bin Yang
Center for Combustion Energy
Tsinghua University
wjxrain@hotmail.com, byang@mail.tsinghua.edu.cn

Zhuyin Ren
Center for Combustion Energy, Tsinghua University
School of Aerospace Engineering, Tsinghua University
zhuyinren@tsinghua.edu.cn

CP16

A Multipurpose Mechanism for Ethanol Combustion

A new and shorter multipurpose skeletal chemical-kinetic mechanism for ethanol combustion comprising 80 reactions and 32 species is presented. Literature survey identifies the state-of-the-art mechanisms to be extensively tested in the wide range of canonical problems representative of technological applications in the combustion science. The benchmark problems are the premixed planar flame propagation (under different equivalence ratio, temperature and pressure), the isobaric autoignition time, and both premixed and non-premixed flame extinction in a counterflow configuration. The selected mechanisms are: The San Diego mechanism (SD), AramcoMech version 2.0, C1-C3 mechanism from The CRECK Modelling group of Milan University (CRECK), Lawrence Livermore National Laboratory (LLNL) and the mechanism developed by MTA-ELTE Research Group of Etvs University (ELTE). The accuracy and computational cost evaluation of above mentioned mechanisms identifies the San Diego Mechanism not only as the most precise mechanism but also as the most convenient option from the point of view of computational cost. Chemistry reduction is achieved by analysing the sensitivity of intermediate species to eliminate the reactions involving the less reactive species. The resulting skeletal mechanism compares favourably with the 235-step, 47 species detailed San Diego Mechanism in all cases studied, reducing the computational cost in more than a 50%.

Alejandro Millán-Merino, Eduardo Fernández-Tarrazo, Mario Sánchez-Sanz
Universidad Carlos III de Madrid
almillan@ing.uc3m.es, eafernan@ing.uc3m.es, mssanz@ing.uc3m.es

CP16

Numerical Simulation of Counterflow Diffusion Flames of Methyl Decanoate Based on a Reduced Mechanism

The growing global demand for energy, along with the environmental, economic and political issues have encouraged the search for energy sources that can replace fossil fuels. In this scenario, the study of oxygenated fuels to reduce engine emissions of CO, NOx, particulate matter and hydrocarbons, gains importance. Biodiesel is produced from vegetable oils or animal fats via the process of transesterification and is an alternative to the diesel derived from oil. Among the advantages of using biodiesel, it is obvious the great capacity of lubrication and the biodegradability. As the composition of biodiesel is too complex to be modeled directly, the studies focus on surrogates, such as Methyl Decanoate (MD), which is a smaller molecule that can reproduce the main features of the combustion of biodiesel. Thus, the present work aims to develop a reduced mechanism for MD, using the techniques of Directed Relation Graph and Sensitivity Analysis. The advantage of using these methods is the elimination of redundant species and reactions, decreasing the computational cost required to solve the equations of chemical kinetics. Numerical simulation is performed in order to validate the reduced mechanism, using the counterflow diffusion flame configuration, and the results compare reasonably with the experimental data available in the literature.

Felipe C. Minuzzi
Federal University of Rio Grande do Sul
felipe.minuzzi@ufrgs.br

Jean Pinho
Federal Institute of Santa Catarina
jean.pinho@ifsc.edu.br

Alvaro De Bortoli
Federal University of Rio Grande do Sul
dbortoli@mat.ufrgs.br

CP16

Performance of Nonstiff and Stiff Chemical Kinetics Integrators on Heterogeneous Processor Architectures

Combustion simulations with finite-rate chemistry rely on accurate and efficient methods for solving stiff ordinary differential equations (ODEs). In a typical reacting-flow solver, the ODEs involving chemical kinetics at each spatial location are decoupled by operator splitting, allowing each to be solved concurrently. Efficient ODE solvers must take into account both numerical efficiency as well as the available thread and instruction-level parallelism of the underlying computational hardware being used to perform the simulations, especially on many-core coprocessors. This talk will summarize work on two complementary efforts to reduce the computational expense of chemical kinetics on modern processing architectures. First, we will examine the performance and behavior of exponential and implicit Runge-Kutta integrators implemented for graphics processing units (GPUs). Second, we will compare the performance of explicit Runge-Kutta and implicit Rosenbrock solvers implemented using both single instruction, multiple thread (SIMT) and single instruction, multiple data (SIMD) paradigms executed on multicore CPUs, Many Integrated Core (MIC), and GPU processors. Lastly, we will make overall conclusions based on a synthesis of the results, and identify remaining open questions and directions for future research.

Nicholas Curtis
University of Connecticut
Department of Mechanical Engineering
nicholas.curtis@uconn.edu

Chris Stone
Computational Science and Engineering, LLC
chris.stone@computational-science.com

Chih-Jen Sung
University of Connecticut

cjsung@engr.uconn.edu

Kyle E. Niemeyer
Oregon State University
Kyle.Niemeyer@oregonstate.edu

CP17

Large Eddy Simulation of Supersonic Combustion in Cavity-Based Scramjet

Due to the low residence time of the flow in high-speed combustors, the flame stabilization in such facilities becomes a real challenge. Cavities are considered as a promising flameholding device as they allow for increasing the residence time of the mixture. However, the resulting flow is complex, featuring supersonic and subsonic regions along with partially premixed combustion. The flame stability depends on both the cavity configuration and the fuel injectors locations. Large eddy simulations are carried out to investigate the stabilization mechanisms at play in such a high speed cavity combustor. The configuration recently studied by Tuttle et al. (JPP 2014) serves as a test-case. In this experimental set-up, velocity measurements (PIV) have been gathered for non-reactive and reactive flows while varying the fuel loading. Simulations are performed using a 9 species and 10 steps reduced kinetic scheme for combustion of ethylene (Singh et al. AIAA Journal 1994). The impact of the choice of the subgrid model for the filtered source terms on the flame dynamics is discussed and a comparison with the available experimental data is provided.

Jiangheng Ruan
CNRS
ruanj@coria.fr

Pascale Domingo
CORIA - CNRS UMR6614
pascale.domingo@coria.fr

Guillaume Ribert
CORIA - CNRS UMR6614
INSA de Rouen
ribert@coria.fr

CP17

An LES-PBE-PDF Approach for Predicting Soot Particle Size Distributions in a Turbulent Diffusion Flame

In many hydrocarbon combustion devices, a major challenge consists in controlling the formation, deposition and emission of soot particles. In this work, we present a comprehensive LES-based model for predicting the evolution of the soot particle size distribution (PSD) in a turbulent flame. From an Eulerian viewpoint, the PSD is governed by the population balance equation (PBE) which accounts for the processes of soot nucleation, growth and, possibly, coagulation. In view of the interaction between turbulence and chemical reactions as well as particle formation, we obtain a transport equation for the joint probability density function (PDF) of the reactive scalars and the particle number density. In practice, expectations with respect to the PDF are approximated by Monte Carlo estimates based on an ensemble of Eulerian stochastic fields whose evolution equations are statistically equivalent to the PDF transport equation. For the discretization along the particle size coordinate, we present an explicit adaptive grid approach which allows resolution in particle size space to be automatically redistributed such that sharp features of the PSD are accurately resolved. Finally, we apply the LES-PBE-PDF model in order to analyze soot formation in the turbulent non-premixed Delft III flame. In the context of this test case, the predictive capability of the model is assessed and the computational efficiency of our numerical solution scheme is demonstrated.

Fabian Sewerin, Stelios Rigopoulos
Imperial College London
Department of Mechanical Engineering
f.sewerin13@imperial.ac.uk, s.rigopoulos@imperial.ac.uk

CP17

Implicit Large Eddy Simulations of Auto-Ignition in a Temporally Evolving Mixing Layer

Strongly unsteady phenomena in reacting flows are regarded as ones of the most difficult problems in contemporary CFD. They involve the interactions between turbulent flow field and emerging turbulent flame being the result of chemical reactions. In this work we will analyse a non-premixed combustion in a temporally evolving mixing layer between streams of a hydrogen and air with a particular attention to auto-ignition and flame propagation. We use a high-order (up to 10th) code which was previously well verified in gaseous shear layer flows with/without chemical reactions. We apply Implicit-Large Eddy Simulation (ILES, Duwig et al., 2011) approach in which we analyse importance of discretization method (TVD, QUICK, WENO, compact-difference) and mesh density on time and localisation of ignition kernel and flame development at the later stage. We compare the results with DNS solutions obtained on very dense meshes and with the LES-CMC simulations. The analysed problem is important both from the fundamental and practical point of view. This work gives deep inside into the mechanism of auto-ignition and we show to what extent it is dependent on physical and numerical (modelling) factors. Among the others it is found that in a case of low temperature difference between the fuel and oxidiser the numerical approach affects the ignition significantly. On the other hand, when the oxidiser temperature is large a modelling of chemical kinetics (mechanism) seems to be a key factor.

Artur Tyliszczak, Agnieszka Wawrzak, Andrzej Boguslawski
Czestochowa University of Technology
Faculty of Mechanical Engineering and Computer Science
atyl@imc.pcz.pl, rosiaka@imc.pcz.pl, abogus@imc.pcz.pl

CP17

Large Eddy Simulations of Explosion Deflagrating Flames Using a Dynamic Wrinkling Formulation

Reliable predictions of flames propagating in a semi-confined environment are vital for safety reasons, once they are representative of accidental explosion configurations. Large eddy simulations of deflagrating flames are carried out using a dynamic flame wrinkling factor model. This model, validated from a priori and a posteriori analysis, is able to capture both laminar and turbulent flame regimes. At early stages of the flame development, a laminar flame propagates in a flow essentially at rest and the model parameter is close to zero, corresponding to a unity-wrinkling factor. Transition to turbulence occurs when the flame interacts with the flow motions generated by thermal expansion and obstacles. The model parameter and wrinkling

factor take higher values at these stages. Three configurations investigated experimentally by Masri et al. (2012) corresponding to different scenarios of flame acceleration are simulated. The first case (OOBS) is characterized by a long laminar phase. In the second one (BBBS) the flame is the most turbulent and the highest overpressure in the vessel is observed. For the last case (BOOS), the flame front is relaminarized after crossing the first row of obstacles. In all configurations, large eddy simulations (LES) predict the flow dynamics and maximum overpressure with good accuracy.

Pedro S. Volpiani
Laboratoire EM2C
CNRS, CentraleSupelec, Université Paris-Saclay
pedro.stefanin-volpiani@ecp.fr

Thomas Schmitt
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr

Olivier Vermorel
CERFACS
vermorel@cerfacs.fr

Denis Veynante
EM2C Laboratory
Ecole Centrale Paris
denis.veynante@ecp.fr

CP17

Large Eddy Simulation of the Inhomogeneous Inlet Jet Flame Using Regularized Deconvolution Method

Recently, a regularized deconvolution method (RDM) has been developed to recover the signal loss in reactive scalars at high wavenumber in large eddy simulation (LES). It is shown that RDM preserves the property of boundedness and conservation of the reactive scalars and the reconstruction procedure is independent of the combustion regimes. In this study, RDM is applied as the closure model for turbulence flame interaction in LES. A posteriori analysis of the model will be conducted for a partially premixed jet flame with inhomogeneous inlets. Both reduced chemistry and tabulated chemistry will be considered in the analysis. The results will be compared against experiment, as well as LES using flamelet progress variable approach (FPVA) and flamelet tabulated chemistry for LES (FTACLES).

Qing Wang
Stanford University
wangqing@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP17

Large Eddy Simulations of a Bluff-Body Stabilized Flame

Bluff-body flame stabilization in premixed flames has been a subject of significant technological interest in gas turbine combustors, afterburners and industrial furnaces. A collaborative computational-experimental effort is reported here, on simulating a series of bluff-body stabilized premixed propane flames near lean blowoff conditions. The numerical models include a large-eddy simulation for the unsteady flow field, a reduced chemical mechanism to account for the finite-rate propane chemistry, as well as a composition transported probability density function method to capture the turbulence-chemistry interactions. Comparison on the mean and rms velocity fields for both the non-reacting flow and the corresponding reacting flow will be made. Parametric studies on the appropriate mixing models to capture the local extinction events will be performed. Finally, the sequence of the physico-chemical events leading to the lean blowoff will be discussed.

Bifen Wu
University of Connecticut
bifen.wu@uconn.edu

Xinyu Zhao
University of Connecticut
Department of Mechanical Engineering
xinyu.zhao@uconn.edu

Bikram Chowdhury, Baki Cetegen
University of Connecticut
bikram.roychowdhury@uconn.edu,
baki.cetegen@uconn.edu

CP18

The Role of Pressure Hessian in Premixed Turbulent Combustion

In turbulent premixed flames, the effects of the turbulent flow field on scalar dissipation transport are dominated by the interplay between scalar gradients and the eigenvectors of the strain rate. Recent work has shown that the pressure Hessian plays an important role in controlling this interplay. In this work, Direct Numerical Simulation databases have been used to investigate the influence of the pressure Hessian on the alignment between scalar gradients and strain rate eigenvectors. These databases cover a range of combustion conditions including the corrugated flamelet and thin reaction zone regimes.

Umair Ahmed
University Of Manchester
umair.ahmed@manchester.ac.uk

Girish Nivarti
Department of Engineering,
University of Cambridge
gvn22@cam.ac.uk

Malgorzata Zimon
IBM Research UK
Daresbury Laboratory
malgorzata.zimon@uk.ibm.com

Robert Prosser
Dept of Mechanical, Aerospace and Civil
Engineering, University of Manchester
robert.prosser@manchester.ac.uk

Stewart Cant
Department of Engineering
University of Cambridge

rsc10@eng.cam.ac.uk

CP18

Flame Structure and Chemiluminescence in Premixed Flames

The quantitative use of chemiluminescence requires the knowledge of the relationship between the concentration of excited species, accessible to measurement, with flame properties such as the equivalency ratio, the burning rate or the heat release rate. With the aim of rigorously finding these relations from first principles, we have analyzed, numerically and analytically, the distribution of the excited chemiluminescent species OH^* and CH^* in steady hydrogen and methane planar premixed flames. The key idea in the analyses, rigorously proven, is that excited OH and CH are in steady state due to their small concentrations. This approach enables the analytical description of the structure of the distribution of both OH^* and CH^* in the flame, revealing how their concentrations are related with other intermediate species, and ultimately of the fuel concentration in the flame. In addition, this approach uncovers and clarifies aspects of the kinetics of premixed flames, which can significantly facilitate the computation of complex turbulent flames.

Jose Grana-Otero
University of Kentucky
jose.grana@uky.edu

CP18

Dynamics of Pulsating Planar Premixed Flames

The unsteady propagation of planar premixed flames in a reactive solid is investigated with the aim of understanding how the dynamics of pulsating fronts depends on the large sensitivity with the temperature of the overall chemical reaction. The unsteadiness is encountered, with a supercritical Hopf bifurcation, after crossing the limit of stability. Close to this limit the oscillations are harmonic with a well defined time scale; but moving deeper into the instability domain these periodic oscillations soon become complicated relaxational-type pulsations, characterized by long stages with front velocities lower than the steady flame velocity, followed by very short stages with very large front velocities. Deeper in the instability domain the propagation becomes chaotic after a series of period doubling bifurcations. For moderately large activation energies of the overall reaction, the usteady flame maintains a classical, quasisteady structure, with a thin reactive layer embedded in reaction-free, unsteady heat-conduction layers. The reactive layers, much thinner than the outer reaction-free layers, are described analytically accounting for the heat conduction losses towards the reacted side of the layer. The problem of the unsteady propagation of the reactive front is then reformulated considering the reaction layer as infinitely thin with appropriate jump conditions. Properties of the soluitons are discussed based on the numerical results

Jose Grana-Otero
University of Kentucky
jose.grana@uky.edu

CP18

Scalar Transport and Damkoehler's Second Hypothesis in the Thin Reaction Zones Regime

The turbulent burning velocity of premixed flames is sensitive to the turbulence intensity of the unburned mixture. Damköhler [Damköhler, G. (1940), *Zeit. Elektro. Chem.*, 46(11):601–652.] put forward two hypotheses concerning the effect of turbulence on the turbulent burning velocity. The first hypothesis applies to low-intensity turbulence which acts mainly to increase the turbulent burning velocity by increasing the flame surface area. The second hypothesis states that, at sufficiently high intensities of turbulence, the turbulent burning velocity is mainly affected by enhanced turbulent diffusivity. Most studies to date have examined the validity of the first hypothesis under increasingly high intensities of turbulence. In the present study, the validity of Damköhler's second hypothesis is investigated. A range of turbulence intensities is addressed using Direct Numerical Simulations spanning the entire Thin Reaction Zones regime. Damköhler's second hypothesis is found to be strongly linked to the response of turbulent transport within the flame.

Girish Nivarti
Department of Engineering,
University of Cambridge
gvn22@cam.ac.uk

Stewart Cant
University of Cambridge
rsc10@cam.ac.uk

CP18

Three-Dimensional Flame-Flame Interaction Topology for Premixed Hydrocarbon Flames

The flame-flame interaction topology for a methane-air flame is analysed using Direct Numerical Simulations (DNS). The DNS configuration consists of two flames propagating towards each other in a field of initially homogeneous and isotropic turbulence. The two flames are allowed to interact freely and a data set containing information on the velocity, temperature, species concentration, pressure and density is obtained. Statistics on all of the possible interaction topologies are extracted and the results are compared with previous data obtained using a hydrogen-air mixture [1] R.A.C Griffiths, J.H. Chen, H. Kolla, R.S. Cant, W. Kollman: Three-dimensional topology of turbulent premixed flame interaction. Proceedings of the Combustion Institute 35, pp. 1341-1348(2014).]. The differences between the statistical results due to the different nature of a hydrocarbon fuel compared to hydrogen are investigated. The implications for modelling of flame-flame interactions within the framework of the flame surface density approach are discussed. A new term in the model may be required to account for the destruction of the flame surface area by the flame-flame interactions.

Shrey Trivedi, Ryan Griffiths
University of Cambridge
st634@cam.ac.uk, racg3@cam.ac.uk

Stewart Cant
Department of Engineering
University of Cambridge
rsc10@eng.cam.ac.uk

CP18

Modelling of Premixed Flames in Progress-Variable Space Including Strain and Curvature Ef-

fects

Originally developed by Peters, flamelet models for non-premixed combustion have been gradually extended and improved in various works in the recent past. In contrary, flamelet models for premixed combustion were only subject to few studies, such as Lodier et al. [1] G. Lodier, L. Vervisch, V. Moureau, P. Domingo, Combust. Flame 158 (2011) 2009 2016.] and Nguyen et al. [2] P.-D. Nguyen, L. Vervisch, V. Subramanian, P. Domingo, Combust. Flame 157 (2010) 43 61.]. In premixed flamelet models the conditioning variable is the progress variable, which is a reactive scalar, as opposed to the passive scalar mixture fraction for non-premixed flamelets. This work shows how to incorporate strain and curvature in the model, which is illustrated by comparison to various well-known flame setups: the planar twin-flame, the planar reactants-to-products and the corresponding tubular flame setups. Additionally, negative strain effects are studied which are in-accessible by conventional, one-dimensional flame setups in physical space, but which occur in turbulent flames. Furthermore, numerical difficulties, that arise when trying to solve flamelet equations in progress variable space, are examined and solution strategies are discussed. With this, this work further develops premixed flamelet models for the eventual usage in CFD in combination with flamelet tabulation strategies.

Axel Zschutschke
TU Bergakademie Freiberg
Numerical Thermo-Fluid Dynamics
axel.zschutschke@iec.tu-freiberg.de

Arne Scholtissek
TU Bergakademie Freiberg
TU Bergakademie Freiberg
arne.scholtissek@iec.tu-freiberg.de

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

CP19

Impact of Reduction of Chemistry on Soot Formation and Evolution in Laminar Flames

The numerical modeling of soot in flames is a numerically challenging and computationally expensive task, requiring the application of detailed kinetic mechanisms able to describe the complex chemistry of aromatic species and soot precursors (such as PAHs). In particular, if the interest is in predicting soot particles in industrial devices or in DNS (Direct Numerical Simulation) of turbulent flows, the complexity of the chemistry must necessarily be sacrificed by considering simplified or skeletal kinetic mechanisms. The objective of this work is to study the impact of such chemical simplifications and reductions on the prediction of formation and evolution of soot in laminar flames. In particular, the analyses have been mainly carried out in 1D laminar diffusion flames, by adopting two different approaches for modeling the formation and evolution of soot particles: i) the Hybrid Method of Moments (Mueller et al. 2009); and ii) the Discrete Sectional Method (Saggese et al. 2015) in which soot chemistry is described through 20 classes of pseudo-species involved in more than 10,000 reactions. Then, the analysis was extended to coflow laminar diffusion flames for which experimental data are available in the literature.

Agnes Livia Bodor
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
agneslivia.bodor@polimi.it

Benedetta G. Franzelli
Ecole Centrale Paris, EM2C CNRS UPR-288
benedetta.franzelli@ecp.fr

Alessandro Stagni, Alberto Cuoci
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
alessandro.stagni@polimi.it, alberto.cuoci@polimi.it

CP19

A New Jet-Stirred Apparatus for Chemical Kinetics Experiments

A novel jet-stirred reactor was designed to study combustion processes at low Damkhler number (Da, ratio of residence time to chemical time), i.e. chemical kinetics. In this new design, multiple impinging turbulent jets are used to stir the mixture. The goal of this work is to identify an optimal configuration of multiple pairs of impinging jets and outlet ports for as a Jet-Stirred Reactor (JSR) for chemical kinetics experiment With this motivation, ANSYS-FLUENT computations using the RANS - Reynolds Stress Model were used to simulate mixing and reaction in such geometries and their performance was compared to classical JSR (4 Jets In Plus (+) Pattern (4JIPP) introduced by Matras & Villermaux 1973; Dagaut et al. 1986; etc.). Results showed that CIAO provided far more uniform composition and temperature and thereby more nearly match the idealizations assumed in well-stirred reactor theory, even at values of Da higher than those accessible to other JSR experiments. Moreover, the CIAO design yielded inferred reaction rate constants that were much to the actual values than the classical JSR design.

Ashkan Davani
University of Southern California
University of Southern California
davanida@usc.edu

Paul Ronney
Univ of Southern California
Dept of Aero. & Mech. Eng.
ronney@usc.edu

CP19

Origins of a Hot Spot for Inhomogeneous End-Gas Autoignition in a Knocking Simulation

A mechanism for the generation of a hot spot for inhomogeneous end-gas autoignition is identified with the results of one-dimensional knocking simulations, where the Navier-Stokes equations are solved with a detailed chemical kinetic mechanism of n-C7H16. The present study demonstrates that a first trigger for the generation of a hot post in end-gas regions is a compression wave generated by the autoignition of an initial high-temperature source. The reflection of the propagating compression wave on the wall produces instantaneous temperature increase, which is significantly higher that that in other end-gas regions. Therefore, some chemical reactions on the wall are promoted compared to those in other end-gas regions with the production of larger amount of key chemical species

such as CH2O and OH. The progress of chemical reactions on the wall steadily continues until the occurrence of low-temperature oxidation and main autoignition whereas the temperature increase is transient, which indicates the formation of a chemically-induced hot spot on the wall.

Hiroshi Terashima
Hokkaido University
htera@eng.hokudai.ac.jp

Akira Matsugi
National Institute of Advanced Industrial Science and Technology (AIST)
a.matsugi@aist.go.jp

CP19

Introducing ChemKED: A New Human and Machine-Readable Data Standard for Chemical Kinetics Experiments

Fundamental experimental measurements of quantities including ignition delay times, laminar flame speeds, and species profiles serve important roles in understanding fuel chemistry and validating chemical kinetics models. However, despite both the importance and abundance of such information in the literature, the community lacks a standard format for this data. This impedes both sharing and wide use by the community. In this talk, we will introduce a new Chemical Kinetics Experimental Data format, ChemKED, and the related Python-based package for creating and validating ChemKED-formatted files called PyKED. We will also review past and related efforts, and motivate the need for a new solution. ChemKED currently supports the representation of autoignition delay time measurements from shock tube and rapid compression machine experiments. ChemKED-formatted files contain all of the information needed to simulate experimental data points, including uncertainty. ChemKED is based on the YAML data serialization language, and is intended as a human- and machine-readable standard for easy creation and automated use. Development of ChemKED and PyKED occurs openly on GitHub. The software is released under the BSD 3-clause license, and contributions from the community are welcome. Plans for future development include extending the ChemKED format and PyKED package to support experimental data for laminar flame speed, jet stirred reactor, extinction, and speciation measurements.

Bryan W. Weber
University of Connecticut
bryan.weber@uconn.edu

Kyle E. Niemeyer
Oregon State University
Kyle.Niemeyer@oregonstate.edu

CP19

Efficient Solution Strategy for the Use of Detailed Chemistry in High-Fidelity Simulations of Turbulent Flames

The use of detailed chemical schemes in high-fidelity simulations of turbulent combustion is essential for the accurate prediction of ignition, flame-stabilization and emissions. The cost of such calculations has long been considered intractable largely due to the small chemical time scale and the expensive source-term calculation. To address these issues, a new integration scheme for the system of ODEs is presented, which is semi-implicit and matrix-free. The resulting efficient ODE solver leads to a direct approach for adaptive kinetics, which focuses on reducing the number of reactions rather than the number of species. Minimal alternation on the existing code is required to adopt these techniques. The so obtained solver has space-time complexity that scales linearly with respect to the number of species. Moreover, the solver is stable in the presence of stiff chemistry and the error introduced by the adaptive kinetics can be strictly controlled. The effectiveness of the techniques is demonstrated in application to various 1D, 2D, and 3D cases.

Hao Wu
Stanford University
wuhao@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP19

Towards Efficient Chemistry Calculations in Combustion Simulations Through Dynamic Adaptive Acceleration

The incorporation of detailed chemistry in combustion simulations is challenging due to the large number of chemical species and the wide range of chemical timescales, which may be further complicated by the transient nature of combustion process. The performance of acceleration methods such as tabulation/retrieval strategies may deteriorate dramatically when large variation in the accessed composition space is presented. In this study, a dynamic adaptive approach is proposed to accelerate chemistry calculations, in which the in situ adaptive tabulation (ISAT) or dynamic adaptive chemistry (DAC) is dynamically selected based on the encountered composition inhomogeneity. The principle component analysis is employed to identify a low-dimensional subspace, in which the composition inhomogeneity of the computational cells is quantified through reconstructing the probability density function of composition in the reduced subspace. ISAT is invoked for regions with high probabilities to avoid unnecessary tabulations that would be rarely reused. DAC is employed to accelerate chemistry calculations for the remaining cells/particles by invoking on-the-fly reduction to generate small skeletal mechanisms for local thermo-chemical conditions. Besides, the consistent error control of ISAT and DAC is also addressed so that only one error tolerance is needed for these two methods. The proposed approach is validated in engine simulations and the performance is analyzed.

Wenwen Xie
Center for Combustion Energy, Tsinghua University
School of Aerospace Engineering, Tsinghua University
jmm15@mails.tsinghua.edu.cn

Zhen Lu
Center for Combustion Energy, Tsinghua University
luz11@mails.tsinghua.edu.cn

Zhuyin Ren
Center for Combustion Energy, Tsinghua University
School of Aerospace Engineering, Tsinghua University

zhuyinren@mail.tsinghua.edu.cn

CP20

Impact of Numerical Discretization and Filter Shape on Large-Eddy Simulations of Turbulent Premixed Flames

Large-Eddy Simulations (LES) provide a computationally feasible approach for representing important time-dependent phenomena associated with reactive flow, such as ignition, shock- and acoustic-related instabilities, and flame blow-out. Of particular importance is the development of suitable sub-grid scale (SGS) models that can correctly capture the above phenomena in compressible reactive turbulence. However, recent studies have highlighted an increased sensitivity to numerical schemes employed in reactive-LES [Cocks et al., Towards Predictive Reacting Flow LES, AIAA 2014-0826]. Addressing such numerical issues is a necessary precursor to SGS model development studies. The present work thus directly considers the impact of the numerical discretization scheme on LES solution accuracy, relative to an explicitly defined filter. Notably, physical model errors are eliminated by providing consistent closure terms, that are derived from an accompanying filtered DNS computation. A statistically planar turbulent premixed flame is considered for cases spanning the corrugated flame and broken reaction zone regimes, and effects of the numerical scheme relative to the LES filter (e.g.: spectral shape, characteristic width) are investigated by means of planar 2D spectra, energy budgets and comparisons to the filtered reference (DNS) solution.

Ayaboe K. Edoh
UCLA
acedoh@gmail.com

CP20

Temperature Consistency Preservation in Large Eddy Simulation-Filtered Mass Density Function (LES-FMDF) Methods for High-Speed Flows

A scalar filtered mass density function method (SFMDF) preserving temperature consistency has been developed for high-speed especially supersonic flows. In this method, the effects of the compressibility and viscous dissipation are added to the source terms of the sensible enthalpy formulation. This method is coupled with LES and implemented through a hybrid Lagrangian Monte Carlo/finite-difference procedure. It is found that the compressible source term for the SMFDF obtained by LES shows obvious errors along discontinuities. To tackle this problem, the concept of particle temperature consistency (PTC) is devised similar to the previous one of particle mass consistency (PMC). The PTC problem is studied and then several primary principles are proposed for LES-FMDF to reach a good consistency even along discontinuities. Based on these principles and other considerations, the source terms of the sensible enthalpy in the FMDF are modeled and computed in a novel perspective. This new LES-SFMDF method is used for simulations of flows in a shock tube and flows in a subsonic temporally developing mixing layer. The new source term calculation method is compared with the previous scheme in the simulations, the results of which show favorable agreement with LES especially when discontinuities exist. This method also demonstrates robustness when various particle numbers are conducted.

Lin Zhang, Jianhan Liang, Mingbo Sun, Hongbo Wang
Science and Technology on Scramjet Laboratory
National University of Defense Technology
zhlin151@163.com, jhleon@vip.sina.com, sunmingbonudt@sina.com, whbwatcn@nudt.edu.cn

CP20

Application of Discontinuous Galerkin Methods for LES Predictions of Turbulent Flames

This talk focuses on the development of a high-order discontinuous Galerkin (DG) method for application to chemically reacting flows. To enable these simulations, several algorithmic aspects are addressed, including the time-integration of multi-step chemical reactions, the incorporation of detailed thermo-viscous transport properties, and the stabilization of high-order solution representation. A scalable parallel DG solver is developed based on this algorithm development and applied to LES predictions of turbulent flame. As an example, this talk will cover the LES study of a turbulent bluff-body stabilized propane/air premixed flame. The simulation results for cold-flow and reacting conditions are reported and compared to experimental data.

Yu Lv
Stanford University
ylv@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP20

The Filtered Wrinkled Flame (FWF) Model for Large-Eddy Simulation of Turbulent Premixed Combustion

Many models for combustion LES, well suited to capture the turbulent flame front displacement speed, do not predict the filtered turbulent flame brush. In this context, this article proposes an analysis of the impact of the flame sub-filter wrinkling level on the filtered flame thickness based on the method of manufactured solutions. Three controlling parameters are identified: i) the flame filter size, ii) the sub-filter flame wrinkling and iii) the number of flame patterns contained within the sub-filter volume. These parameters are well defined and several models are available in the literature for the two latters. Then, a new turbulent combustion model is proposed following this concept: The Filtered Wrinkled Flame (FWF) model estimates the unclosed terms of the filtered progress variable equation by explicitly filtering 2-D wrinkled flames for different filter sizes and different wrinkling levels. An a priori validation is conducted by comparing the sub-filter PDF provided by the model to an existing DNS database. An a posteriori validation is then performed on 1-D filtered flames and in the Large-Eddy Simulation (LES) of a semi-industrial swirl burner and of a pulsed turbulent premixed flame anchored at a triangular flame holder. Results are in good agreement with the experiments and validate the proposed methodology. The influence of the flame pattern period at the sub-filter scale is observed and discussed.

Vincent R. Moureau
CORIA Laboratory - CNRS UMR6614
Université et INSA de Rouen
vincent.moureau@coria.fr

Renaud Mercier

SAFRAN Tech, France
renaud-c.mercier@safrangroup.com

Benoit Fiorina
Laboratoire EM2C, Ecole Centrale Paris
benoit.fiorina@centralesupelec.fr

CP20

Sub-Grid Scale Modeling of the Equation of State for Fully Compressible Combustion LES

In Large Eddy Simulation of multicomponent and fully compressible flows, formally the pressure is obtained after filtering the equation of state. In practice, correlations between density, species and temperature are usually neglected to compute the filtered pressure from the resolved fields. The conditions under which this hypothesis is valid are discussed from simulations of hydrogen-oxygen combustion performed with a fully compressible flow solver (SiTCom-B), including detailed chemistry and complex transport. Analysing one-dimensional and three-dimensional H2/O2 space- filtered flames, it is found that a large part of the error introduced by the linearization of the equation of state can be counterbalanced by expressing the mean molar weight of the mixture with the Reynolds filtered species mass fractions, instead of the density weighted ones. An approximate deconvolution/filtering procedure is then discussed to estimate the Reynolds filtered mass fractions from the density weighted mass fractions, which are the transported quantities in LES flow solvers.

Guillaume Ribert
CORIA - CNRS UMR6614
INSA de Rouen
ribert@coria.fr

Pascale Domingo
CORIA - CNRS UMR6614
pascale.domingo@coria.fr

Luc Vervisch
INSA Rouen CNRS CORIA
vervisch@coria.fr

CP20

Impact of Radiation Modeling in Large Eddy Simulation of a Turbulent Sooting Diffusion Ethylene-Air Flame

Soot modeling is today recognized as an extremely challenging problem in turbulent combustion due to the strong interactions between turbulence, chemistry and particles. In addition, a non-linear coupling exists between soot and radiation due to the high radiative contribution of soot to the total heat transfer.
A Large Eddy Simulation of a turbulent sooting diffusion flame is performed based on state-of-art modeling for the gaseous phase, using a non-adiabatic flamelet progress variable approach combined with a relaxation model for PAHs, and for the solid phase, employing a detailed sectional model with a subgrid model accounting for intermittency. For simplicity and to reduce the computational cost, the optically thin model is generally considered for both gaseous and solid phases. The objective here is to identify the impact of this assumption by using a Monte-Carlo solver, which accounts for the re-absorption phenomenon by solving the radiative transfer equation, and provides a detailed description of radiative properties: (1) a detailed CK-model for the gaseous phase; (2) a wavelength-dependent refractive index and morphological dependent radiative properties for soot particles.
For each step, results on temperature and soot volume fraction are compared to the optically thin solutions and to experimental data, the different radiative contributions are quantified and impacts on both quantities are evaluated.

Pedro Rodrigues
Laboratoire EM2C, CNRS, CentraleSupélec,
Université Paris-Saclay
pedro.rodrigues@centralesupelec.fr

Ronan Vicquelin
EM2C, CNRS, Ecole Centrale Paris
ronan.vicquelin@centralesupelec.fr

Benedetta G. Franzelli
Ecole Centrale Paris, EM2C CNRS UPR-288
benedetta.franzelli@ecp.fr

Olivier Gicquel, Nasser Darabiha
EM2C Laboratory
Ecole Centrale Paris
olivier.gicquel@ecp.fr, nasser.darabiha@ecp.fr

CP21

Eulerian-Lagrangian Simulation of Non-Spherical Biomass Particles in Turbulent Flow

Most of the current computation fluid dynamics (CFD) simulations of biomass combustion and gasification treat pulverized biomass particles as spherical particles with either same diameter or same equivalent volume. However, pulverized biomass particles as employed in gasification and combustion furnaces are typically highly non-spherical. From non-reacting flow simulations it is shown that the predominant elongated needle-like biomass particles have unique trajectories affecting also thermodynamics properties in the furnace. Thus, CFD simulation results with the spherical particles assumption may differ significantly from what is found in experiments. In this work, an ellipsoidal point-like particle model has been implemented into the open source CFD platform OpenFOAM to investigate the velocity and spatial distribution of biomass particle in turbulent reacting channel flow.

Ning Guo, Tian Li
Norwegian University of Science and Technology (NTNU)
ning.guo@ntnu.no, tian.li@ntnu.no

Terese Lovas
Norwegian University of Science and Technology
terese.lovas@ntnu.no

CP21

Collaborative Simulations and Experiments for Development and Uncertainty Quantification of a Reduced Char Oxidation and Gasification Model in Oxy-Coal Combustion Conditions

The development of reduced physics models with quantified model-form uncertainty is desirable to overcome the challenges of performing LES of industrial coal-fired boilers. Reduced models must ensure the main features of the detailed models and the capability of bridging different scales and being predictive. A tight coupling of sim-

ulation and experiments is necessary to ensure predictivity with uncertainty quantification for a reduced model. This work proposes a combined experimental/numerical methodology that uses data collaboration to derive a reduced char-combustion model describing reactions between chars carbon and O2, CO2 and H2O reagents in oxy-coal conditions. A valuable evaluation of uncertainty in the data, in the model form and in the model parameters has been performed. The dataset is provided by the experiments carried out in a laminar entrained flow reactor operated by Sandia National Laboratories. The methodology involves the use of so-called instrument models to include all the physical sub-models and the sources of uncertainty considered in the experiments and in the numerical simulations and affecting the main quantities of interest, e.g. reaction rates. The quantified uncertainty in the instrument models provided the range of uncertainty for the reduced char combustion model. Then, the reduced model with quantified uncertainty has been validated against the experimental data.

Salvatore Iavarone
Université Libre de Bruxelles
Salvatore.Iavarone@ulb.ac.be

Benjamin Isaac
Institute for Clean and Secure Energy, University of Utah
bisaac2@gmail.com

Sean Smith
The University of Utah
sean.t.smith@utah.edu

Philip J. Smith
University of Utah
Philip.Smith@utah.edu

James Oreluk
University of California Berkeley
jim.oreluk@berkeley.edu

Andrew Packard
U of California at Berkeley
apackard@berkeley.edu

Michael Frenklach
University of California at Berkeley
myf@me.berkeley.edu

Alessandro Parente
Université Libre de Bruxelles
alparent@ulb.ac.be

CP21

Scalar Gradient Statistics for Regime Independent Modeling

One of the few modeling approaches of turbulent combustion that have the promise of being regime-independent is the transported probability density function (TPDF) method. A central unresolved issue with the TPDF methods is the modeling of the mixing term that requires a closure of a reacting scalar dissipation rate as well as a mixing rule. A method based on the joint PDF of the scalar and its gradients is proposed here to provide a closure for the scalar dissipation rate. The resulting TPDF equation encapsulates the influence of the turbulence mixing and the chemical reactions on the evolution of the scalar gradient in separate terms. Therefore, the interplay between the two can be systematically captured across regimes spanning low to high Damkohler numbers. An a-posteriori study is performed to assess the scalar gradient joint T-PDF modeling using statistically one-dimensional turbulent premixed flame DNS data sets. The DNS data sets are chosen to span the corrugated and thin reaction zones regimes in multiple configurations. The a-posteriori assessment is systematically performed by gradually expanding the terms that are modeled versus those that are provided from the DNS.

Hemanth Kolla
Sandia National Laboratories
hnkolla@sandia.gov

Hasret Turkeri
Department of Mechanical Engineering
University of Connecticut
xinyu.zhao@uconn.edu

Xinyu Zhao
University of Connecticut
Department of Mechanical Engineering
xinyu.zhao@uconn.edu

CP21

Eulerian-Lagrangian Simulation of Thermochemical Degradation of Thermally Thick Biomass Particles

Devolatilization is a crucial step in the processes of thermal-chemical conversion of biomass. Thermal degradation of the biomass are influenced by whether the particles are thermally thick or thin. Due to the inherent physical properties, it is difficult to prepare small particles of biomass especially for the lignocellulosic biomass. Therefore, temperature gradients within biomass particles should also be considered when simulating high-temperature conversion of biomass. In this study, a computation fluid dynamic (CFD) model is developed to simulate thermochemical degradation of biomass particles in a wide range of Biot number. A particle sub-model proposed by Strm and Thunman has been implemented into an existing Eulerian-Lagrangian CFD model within the OpenFOAM framework. The particle sub-model resolves the gradients of temperature and species inside a particle with three distinct layers: moist wood, dry wood, and char. It is found that depending on the Biot number of biomass particle, temperature gradients inside particle vary differently. For the particle with a large Biot number, significant temperature gradients lead to the simultaneous drying and devolatilization. Such phenomenon is not possible to be predicted with the assumption of zero temperature gradients inside particle, which is usually applied in the Eulerian-Lagrangian CFD model. The developed CFD model is also examined by a detailed comparison with experimental data.

Tian Li
Norwegian University of Science and Technology (NTNU)
tian.li@ntnu.no

Terese Lovas
Norwegian University of Science and Technology
terese.lovas@ntnu.no

CP21

Improvements to Photon Monte Carlo Radiation

Solver for Combustion Simulations

Importance of accurate radiation modeling in combustion is often undermined by the computational complexity of radiation solvers. The photon Monte Carlo (PMC) method with line-by-line (LBL) spectral data provides the most accurate and robust radiation solver. But PMC/LBL has high computational cost due to ray tracing and large memory requirements due the LBL database (of the order of few GB per processor). In this work we present three novel techniques to improve time and memory requirement for PMC/LBL in combustion simulations with parallel scalability in mind. The first improvement utilizes a POSIX memory map (MMAP) based parallel memory management algorithm, where the LBL database is accessed only on a need-to-know basis and is shared efficiently across processors. The advantage of this method increases with the number of processors per core. The second improvement is a deferred ray tracing approach for PMC, which reduces the granularity of data transfer across processor boundaries at each time step, thereby increasing parallel efficiency. The third improvement introduces a new algorithm for interaction between rays and participating media, if the medium is modeled using a Lagrangian framework. Preliminary results suggest roughly a factor of three reduction in memory requirement per processor in parallel runs, at least 15% increase in scaling efficiency, and significant improvement in computational time for ray-medium interactions.

Somesh P. Roy
Department of Mechanical Engineering
Marquette University
somesh.roy@marquette.edu

Steffen Weise
TU Freiberg
steffen.weise@iec.tu-freiberg.de

Ankur Gupta
FM Global
ankur.gupta@fmglobal.com

Michael Modest
University of California Merced
mmodest@ucmerced.edu

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

Daniel C. Haworth
Pennsylvania State University
dch12@psu.edu

CP21

Systematic Error Analysis and Error Reduction of Interpolation-Based Moment Methods (MOMIC/HMOM) for Statistical Soot Modeling

Interpolation-based moment methods such as the Method of Moments with Interpolative Closure and the Hybrid Method of Moments are widely used statistical approaches to describe aerosol dynamics such as soot evolution. When performing numerical simulations, typically transport equations are solved for a few low order integer moments of the soot Number Density Function, and fractional or negative order moments required for closure are obtained via interpolation or extrapolation. The errors induced by such procedures are studied in a combination of a priori and a posteriori analyses using Monte Carlo simulations as reference solution. The effect of solving an additional equation for the moment of order minus infinity to replace the extrapolation of negative order moments by an interpolation is analyzed. It is further discussed why particularly the evaluation of moments of orders between zero and one represents a challenging task and may result in a systematic overprediction of the soot surface growth term, and why increasing the order of the interpolation polynomial does not resolve this issue. Based on these considerations, an alternative scheme for the evaluation of fractional moments is proposed, which leads to reduced errors in the fractional moments and hence in the soot source terms. This error analysis and reduction is first performed for a univariate soot model based on particle volume, and then extended to a bivariate model based on volume and surface area.

Achim Wick, Manish Kumar
Institute for Combustion Technology
RWTH Aachen University
a.wick@itv.rwth-aachen.de, manish030297@gmail.com

Heinz Pitsch
Aachen University
h.pitsch@itv.rwth-aachen.de

CP22

Direct Numerical Simulation of Premixed Turbulent Jet Flames at High Reynolds Number

A set of direct numerical simulations of turbulent premixed jet flames at different Reynolds and Karlovitz numbers is presented. The gas phase hydrodynamics are modeled with the reactive, unsteady Navier-Stokes equations in the low-Mach number limit. The simulations feature finite rate chemistry with 16 species and 73 reactions and up to 22 Billion grid points. The jet consists of a methane/air mixture with equivalence ratio $\phi = 0.7$ and temperature varying between 500 and 800 K. The temperature and species concentrations in the coflow correspond to the equilibrium state of the burnt mixture. All the simulations are performed at 4 atm. The flame length, normalized by the jet width, decreases significantly as the Reynolds number increases. This is consistent with an increase of the turbulent flame speed due to the increased integral scale of turbulence. This behavior is typical of flames in the thin-reaction zone regime, which are affected by turbulent transport in the preheat layer. Fractal dimension and topology of the flame surface, statistics of temperature gradients, and flame structure are investigated and the dependence of these quantities on the Reynolds number is assessed.

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Stefano Luca
King Abdullah University of Science and Technology
stefano.luca@kaust.edu.sa

Fabrizio Bisetti
University of Texas at Austin, USA
fbisetti@utexas.edu

CP22

Direct Numerical Simulations of Spherically Ex-

panding Turbulent Premixed Flames

Three-dimensional direct numerical simulations of methane-air premixed spherically expanding flames in homogenous isotropic turbulence are conducted to characterize the response of the propagating flame to turbulence over a range of Reynolds numbers. This configuration is chosen due to its simplicity and opportunity for comparison with experiments. A methane/air mixture with an equivalence ration of 0.7 is considered at 4 atm with an unburnt temperature of 800K. The gas phase hydrodynamics are modeled with the reactive, unsteady Navier-Stokes equations in the low Mach number limit. A newly developed skeletal kinetic mechanism, which includes 16 species and 73 elementary reactions, is used to represent methane/air reactions. Temperature dependences of transport and thermal properties are also considered. Simulations with turbulent Reynolds numbers varying between 60 and 220 and meshes up to 8 billion points are performed. Turbulent flame speeds and mean flame brush thickness are analyzed together with local flame structure and the effect of turbulence and pressure are quantified.

Romain Buttay
Physical Sciences and Engineering Division
King Abdullah University of Science & Technology
romain.buttay@kaust.edu.sa

Stefano Luca
King Abdullah University of Science and Technology
stefano.luca@kaust.edu.sa

Ravi Samtaney
KAUST
ravi.samtaney@kaust.edu.sa

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Fabrizio Bisetti
University of Texas at Austin, USA
fbisetti@utexas.edu

CP22

Direct Numerical Simulation of Flame Stabilization over a Rectangular Cavity with Compressibility Effects

Flame stabilization in scramjet combustors, which possess short residence times of the order of 0.1 ms, is often achieved using a cavity flame holder that recirculates hot products of combustion including radicals. In the present study direct numerical simulations (DNS) are performed to understand the stabilization of a lean ethylene-air premixed flame in the shear layer above a rectangular cavity. The DNS are performed with S3D using a compressible formulation of the Navier-Stokes equations coupled with a reduced chemical model for ethylene-air with 22 transported species. A premixture of ethylene-air at an equivalence ratio of 0.4 is advected into the domain at a Mach number of 0.6. Both laminar and turbulent profiles at the inflow are considered in the DNS. Flame stabilization is found to be significantly affected by the shear flow dynamics between the main flow and the cavity flow, while the recirculation flow pattern within the cavity is dictated by its aspect ratio. The stabilization mechanism is quantified in terms of relevant non-dimensional parameters and statistics will be presented regarding the detailed interaction between the flame and flow structures.

Aditya Konduri
Sandia National Laboratories
akondur@sandia.gov

Andreas Rauch
University of Virginia
ahr6wa@virginia.edu

Hemanth Kolla
Sandia National Laboratories
hnkolla@sandia.gov

Harsha Chelliah
University of Virginia
hkc3w@eservices.virginia.edu

Jacqueline Chen
Combustion Research Facility
Sandia National Laboratories
jhchen@sandia.gov

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

CP22

Direct Numerical Simulations of Forced Ignition Behind a Backward Facing Step in Subsonic Flow

A backward facing step (BFS) is a canonical configuration used to investigate flow separation which may lead to recirculation and vortex shedding. These features are relevant to a wide range of engines such as gas turbines and RAM/SCRAM jet engines where flame holding (e.g., via recirculating flow) is required to initiate and sustain combustion at high speeds and short residence times. In the present direct numerical simulation study, subsonic flow over a two-dimensional BFS is used to study the process of flame stabilization/blow-off following forced ignition. A mean turbulent inlet profile with premixed reactants was selected in order to isolate the unsteadiness caused by the mean flow from the influence of turbulent fluctuations and fuel stratification. After the flow becomes fully-developed, periodic vortices are shed and advected out of the domain. The vortex shedding introduces unsteadiness that affects the size of the recirculation zone and the location of the flow reattachment. Ignition kernels are imposed on the developed flow and several parametric variations are conducted that investigate the interactions between the ignition kernel and mean flow unsteadiness. The nature of these interactions aid in defining ignition success criteria. Ignition success is found to depend upon many factors, including: ignition timing, ignition location, ignition energy, equivalence ratio, and vortex-to-vortex variability.

Alex Krisman
Combustion Research Facility
Sandia National Laboratories
ankrism@sandia.gov

Aditya Konduri
Sandia National Laboratories
akondur@sandia.gov

Jacqueline Chen
Combustion Research Facility

Sandia National Laboratories
jhchen@sandia.gov

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

CP22

Direct Numerical Simulation of Two-Phase Flows with Phase Change in Subcritical and Supercritical Regimes

This study introduces a method to treat interfaces in a multiphase flow with phase changes conserving typical Direct Numerical Simulation (from the turbulence point of view) resolution while its applicability to Large-Eddy Simulation is under investigation. This method allows the simulation of such flows with real gas thermodynamics for a wide range of regimes, from a subcritical two phase flow where the capillary dynamics pilot the system through the surface tension to a supercritical fluid where such effects disappear. The thermodynamic consistency of the method, a key element, has been thoroughly investigated and demonstrated using canonic mono-dimensional cases. The model is shown to adapt to the regime, to perfectly retrieve the saturation values and to capture and preserve the interface dynamics, without the need of any additional ad-hoc information. This method has been implemented in the code AVBP, developed by CERFACS and IFPEN, to perform two-dimensional simulations and has been validated trough the study of the dynamics of droplets out of equilibrium. Finally, going towards applicative cases such as cryogenic rocket jets, the model has been used to simulate a mixing layer between two phases with a transition between subcritical and supercritical regimes.

Davy Nayigizente
EM2C Laboratory
davy.nayigizente@ecp.fr

Thomas Schmitt
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr

Sébastien Ducruix
EM2C Laboratory
sebastien.ducruix@centralesupelec.fr

CP22

Direct Numerical Simulation of Particle Burning for Pulverized Coal Combustion

Pyrolysis, volatile ignition and char conversion strongly affect the characteristics of pulverized coal combustion (PCC). We perform three-dimensional Direct Numerical Simulation (DNS) of the pyrolysis and combustion of particles undergoing PCC, resolving all relevant flow and flame scales and providing detailed information on small-scale processes which occur on the sub-grid of Large Eddy Simulations (LES). In our DNS pyrolysis is described by a generic boundary condition at the particle surface that accounts for both convective and diffusive phenomena. Subsequent to pyrolysis, heterogeneous reactions are considered, accounting for CO/O2 production/consumption rates at the particle surface. The heating rate history of the particle is obtained by solving for intra-particle heat transfer and heat exchange between the particle and its surroundings. The time evolution of volatile release is captured by using the particle temperature to calculate the pyrolysis rate from a single kinetic rate law with CPD-fitted parameters. In the DNS pyrolysis and combustion of selected particles from an LES of the semi-industrial IFRF coal furnace #1 are characterized. The LES provides particle number density, particle trajectory, velocity statistics, turbulence scales and surrounding gas composition for the DNS. In turn, the DNS is performed on a computational domain of typical LES cell size and yields crucial sub-grid information to improve PCC-LES models.

Oliver T. Stein
Stuttgart University
Institute for Combustion Technology
oliver.stein@itv.uni-stuttgart.de

Giovanni-Luigi Tufano, Andreas Kronenburg
Institute for Combustion Technology (ITV)
Stuttgart University
itvgt@itv.uni-stuttgart.de, itvak@itv.uni-stuttgart.de

Martin Rieth
University of Duisburg-Essen
martin.rieth@uni-due.de

Andreas Kempf
Duisburg-Essen University
andreas.kempf@uni-due.de

Michele Vascellari
Virtuhcon, Chair of Numerical Thermo-Fluid Dynamics
TU Freiberg
Michele.Vascellari@vtc.tu-freiberg.de

Christian Hasse
Technische Universitaet Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
christian.hasse@iec.tu-freiberg.de

CP23

Soot Formation Prediction of the Combustion Field of 4 KW Pulverized Coal Jet Burner by the Large Eddy Simulation with the Tabulated-Devolatilization-Process (TDP) Model

Pulverized coal combustion is used in the majority of coal-fired thermal power plants. To operate the coal-fired thermal plants efficiently and to reduce the emissions of environmental pollutants, the understandings of the phenomena inside the furnace is important. Since it is difficult to measure the temperature and chemical species concentrations and particle behaviors inside the actual large scale furnace for the understandings of the phenomena inside the furnace, the numerical simulation has been expected to be useful tool for obtaining such information inside the furnace. In particular, the large eddy simulations (LES) have been employed for the prediction of coal combustion field by some researchers to improve the calculation accuracy. Soot particle is one of the most important intermediate substance in the coal combustion field. However, soot particle formation has not been considered in most LES of the coal combustion field. In this study, the soot formation in the coal combustion field was predicted by LES with the tabulated-devolatilization-process (TDP) model. The predicted soot volume fraction distributions were compared with the measured data. The results showed that the LES could reproduce the soot volume fraction distributions in

the coal combustion field.

Nozomu Hashimoto, Hiroyasu Takahashi
Hokkaido University
nozomu.hashimoto@eng.hokudai.ac.jp,
hiroyasu@eis.hokudai.ac.jp

Hiroaki Watanabe
Department of Mechanical Engineering
Kyushu University
whiroaki@mech.kyushu-u.ac.jp

Ryoichi Kurose
Kyoto University
kurose@mech.kyoto-u.ac.jp

Osamu Fujita
Hokkaido University
ofujita@eng.hokudai.ac.jp

CP23

Turbulent Reacting Hydrogen-Enriched Methane-Oxy Flames in a Swirl-Stabilized Gas Turbine Combustor

The study presents numerical investigation of oxy-combustion H2-enriched-CH4 diffusion flames in an atmospheric pressure swirl stabilized gas turbine model combustor. The flames characteristics in terms of temperature and species distributions, structures and flow fields are studied numerically over ranges of operating parameters. The effects of equivalence ratio, oxidizer composition, H2-enrichment and swirl vane angle on flame stability, temperature distribution and flow field are studied in details. The swirl number considered is 1.10 with corresponding swirl vane angle of 55o. ANSYS Fluent was used to perform the numerical study and the models adopted are; k-e (standard), discrete ordinate (DO), eddy-dissipation-concept (EDC) for turbulence, radiation, and species transport. Combined modified Jones-Lindstedt reaction mechanism and Marinov reaction mechanism for H2 were considered as reaction mechanism for the numerical study. The numerical results are in good agreement with their corresponding experimental data. It was observed that utilizing H2enriched-CH4 improves the flame stability. The numerical results showed that oxy-fuel combustion of H2-enriched-CH4 is not achievable at an equivalence ratio of 0.95 and above due to stability issues. The stability is highly enhanced by the corresponding formation of inner recirculation zone. A swirler with swirl vane angle of 65o achieved better stability limits of the gas turbine combustor.

Medhat A. Nemitallah
King Fahd University of Petroleum and Minerals
medhatahmed@kfupm.edu.sa

Mohamed Habib, Syed Said, Mansur Aliyu, Sherif Seif Eldin
King Fahd University of Petroleum and Minerals
Dhahran, Saudi Arabia
mahabib@kfupm.edu.sa, smasaid@kfupm.edu.sa, g201404960@kfupm.edu.sa, sherifs@kfupm.edu.sa

CP23

Dynamics of a Transcritical Coaxial Flame Submitted to Fuel Injection-Rate Modulations: Analysis of the Generation of Heat-Release Rate Unsteadiness and Low-Order Modeling

The present study is motivated by the need for improved understanding and modeling capabilities for high-frequency combustion instabilities in liquid-rocket engines. It is established that acoustic pressure fluctuations within the combustion chamber or the engines feeding system can induce temporal modulations of the propellants injection velocities. The dynamic response of a transcritical coaxial flame to such velocity modulations is here investigated through large-eddy simulation (LES). The annular fuel stream is acoustically modulated at several frequencies. It is shown that the heat-release rate distribution is highly correlated to the flame stretch rate perturbations induced by the modulation. The temporal response of the total heat-release rate strongly depends on the modulation frequency and a classical low-pass behavior is observed for the response amplitude. The phase-lag proves to evolve linearly with the modulation frequency. The thermo-acoustic contribution to the acoustic energy budget depending largely on the heat-release rate/pressure phase-lag, this mechanisms phase-lag is then one of the key parameters for the prediction of combustion instabilities. A low-order model that reproduces this mechanism is proposed, and the resulting model transfer function is successfully confronted to the flame transfer function samples obtained from the various LES computations.

Robin Nez
Laboratoire EM2C, CNRS UPR288, CentraleSupélec, Université Paris-Saclay
robin.nez@ecp.fr

Thomas Schmitt
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr

Manuel Gonzalez-Flesca
1) Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay 2) CNES DLA
manuel.gonzalez-flesca@ecp.fr

Sébastien Candel
Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay
sebastien.candel@ecp.fr

Sébastien Ducruix
EM2C Laboratory
sebastien.ducruix@centralesupelec.fr

CP23

A Numerical Study of Hot Spot Ignition at Rapid Compression Machine Conditions

Non-uniform, or mild ignition, can sometimes be observed during rapid compression machine and shock tube experiments. This form of ignition can be caused by, among other things, thermal inhomogeneities, which lead to flame kernel initiation, growth and propagation. The end(wall) gas can be compression heated by the propagating flame until autoignition ensues. This is observed in the pressure records as a slow pre-ignition heat release leading to shortened ignition delay times, as well as optically via schlieren techniques and natural chemilluminescence direct observation of heterogeneous flame propagation. Simulations in the present study systematically investigate effects of thermal inhomogeneities on syngas ignition behavior at conditions where mild ignition has been observed in experiments.

Mild ignition is found to be affected by properties of the mixture (homogeneous ignition, laminar flame speed, thermal and mass transport) as well as the size and intensity of thermal inhomogeneities, which can be influenced by the operating characteristics of the facility.

Jeffrey Santner
Argonne National Laboratory
jsantner@anl.gov

CP23

Numerical Investigation of Flame Flashback in an Ethylene-Fueled Scramjet Combustor at Mach 5.5 Flight Condition

Flame flashback inside an ethylene-fueled scramjet combustor is investigated in Mach 2.52 facility with the stagnation temperature of 1460K. The equivalence ratio f of ethylene is 0.24. Experimental data suggests that the flame flashback process contains strong flame triggering and flame flashback. Fuel injection upstream of the cavity flameholder produces a premixed region and a rapid flame flashback occurs against the incoming supersonic flow. The flashback develops explosively from the cavity pilot flame at regular intervals. For numerical comparison, three inflow boundary layer thickness, d=0mm, 1.5mm and 3mm respectively was considered. Simulation suggests that cavity strong flame triggering is related to the interaction of the jet plume with the cavity downstream flow. For d=1.5mm and 3mm, strong flame is triggering and moves back to fuel jet while flame stays in the cavity shear layer all the time for d=0mm. The observed flame triggering is much easier for thick boundary layer since the turbulence level is increased downstream of the cavity aft wall as the inflow boundary layer thickness increases. Flame spreads along a fuel/air premixed region from the injection to the cavity flameholder and demonstrates a fast flame flashing-back process. The pre-combustion shock is pushed upstream and interacts significantly with the boundary layer, which provides a more appropriate low-speed and high temperature region for flame flashback.

Mingbo Sun
Science and Technology on Scramjet Laboratory
National University of Defense Technology
wind_flowcfd@163.com

Jinshui Wu, Xingda Cui
Science and Technology on Scramjet Laboratory, National Univ
nudtwjs@126.com, xingdacui@163.com

Hongbo Wang
National University of Defense Technology
whbwatch@nudt.edu.cn

Jianhan Liang
Science and Technology on Scramjet Laboratory, National Univ
jhleon@vip.sina.cn

CP23

Numerical Study on Combustion Structure in a Cavity-Based Supersonic Combustor

Large eddy simulation (LES) has been carried out to investigate a supersonic combustor with hydrogen injection upstream of a cavity flameholder, where a Reynolds-Averaged Navier-Stokes (RANS) model is used for near-wall treatment. The results indicate that both autoignition and flame may be significant in this cavity-stabilized combustion with moderate total temperature (1486K). In the interactional regions between the fuel jet and the cavity shear layer, autoignition first occurs in the partially premixed regions within/under the fuel jet and then evolves into premixed flames that are stabilized by the cavity. Thus, the combustion around the cavity corresponds to that of autoignition-assisted premixed flames. The oxygen in the near-wall regions is then consumed quickly by these fuel-rich premixed flames so that only the surplus fuel and combustion products/radicals exist within/under the fuel jet in the zone downstream of the cavity, where diffusion flames are formed in the periphery of the fuel jet and stabilized by the upstream premixed combustion. Moreover, the simulation shows that temperature and velocity fluctuations levels can reach up to 20% – 40% while species fluctuations levels may be higher.

Hongbo Wang
National University of Defense Technology
whbwatch@nudt.edu.cn

Mingbo Sun, Chaoyang Liu, Peibo Li
Science and Technology on Scramjet Laboratory
National University of Defense Technology
wind_flowcfd@163.com, chaoyangliucn@1, lipeibo@hotmail.com

CP24

A New Jet-Stirred Apparatus for Turbulent Premixed Flame Experiments

A new jet-stirred chamber (JSC) design incorporating multiple impinging turbulent jets is proposed as an apparatus for the study of turbulent premixed flames. ANSYS-FLUENT computations employing the RANS - Reynolds Stress Model were used to simulate the flows and identify an optimal configuration of jets and outlet ports providing the most nearly ideal flow, i.e. homogeneous and isotropic with large turbulence intensity compared to the mean velocity. Results showed that a configuration of 8 jets, each surrounded by a concentric annular outlet, at the corners of an imaginary cube circumscribed by a spherical chamber produced by far the most nearly optimal flow characteristics. The performance of this configuration, called Concentric Inlet And Outlet (CIAO), was also compared quantitatively to two popular fan-stirred chamber (FSC) designs and CIAO JSC was found to provide far more nearly ideal flow. A comparison of simulated turbulent premixed flames at high Damkhler numbers (Da, ratio of chemical reaction rate to turbulent strain rate) in CIAO and an FSC showed that CIAO enabled far more nearly spherical expanding flames with nearly the same inferred turbulent burning velocity regardless of the value of the mean progress variable used to define the flame location, whereas in the FSC there was considerable variation depending on the definition.

Ashkan Davani
University of Southern California
University of Southern California
davanida@usc.edu

Paul Ronney
Univ of Southern California
Dept of Aero. & Mech. Eng.

ronney@usc.edu

CP24

Three-Dimensional Linear Eddy Modelling of Turbulent Hydrogen Jet Flames in Co-Flow

Continuing the work of Sannan et al. [Flow Turb. Combust., 2013, 90 : 189 − 216], a 3D modelling approach based on the Linear Eddy Model (LEM) is presented and verified. The needed fidelity is achieved through a reduced physical/mathematical description of turbulence and its interactions with chemical reactions.
Structurally, LEM3D involves a 3D lattice-work of orthogonal arrays of LEM domains. The spacing of the LEM domains within this structure is coarse and is intended to capture large-scale 3D effects through domain coupling. As in 1D LEM, this formulation involves spatial rearrangements of fluid elements (control volumes in a finite-volume interpretation), but extended to include transfers of fluid elements between, as well as within, LEM domains. Thereby LEM3D also maintains the strict segregation of advective and molecular diffusive time advancement, which provides maximum fidelity for combustion applications.
In the current work, the in-house LEM3D code with full implementation of the CHEMKIN library and parallelization, to allow sub-cycling of LEM domain advancement, is completed. The code has been coupled to the state-of-the-art flow solver, ANSYS FLUENT and shows that the coupled RANS-LEM3D tool has the potential of direct industrial application with the allowance for complex geometries such as in gas turbine combustors.
The model has been validated using experimental and numerical data from lifted turbulent hydrogen jet flames in a vitiated co-flow.

Fredrik Grøvdal
Norwegian University of Science and Technology(NTNU)
fredrik.grovdal@ntnu.no

Sigurd Sannan
SINTEF Energy Research
sigurd.sannan@sintef.no

Alan Kerstein
Consultant
alan.kerstein@gmail.com

J.Y. Chen
U.C. Berkeley
jychen@euler.berkeley.edu

Terese Lovas
Norwegian University of Science and Technology
terese.lovas@ntnu.no

CP24

Comparisons of Flame Surface Density Measurements with Direct Numerical Simulations of a Lean Methane-Air Flame in High-Intensity Turbulence

The turbulent burning velocity of premixed flames exhibits a non-linear variation under increasing turbulence intensity of the unburned mixture. This phenomenon, known as the bending effect, has not been fully explained to date. A key aspect is the mechanism responsible for the observed departure from linearity. Experimental measurements of spherically-expanding flame kernels [Bradley et al. (2013), *Proc. Combust. Inst.*, 34:1519–1526.] point towards local quenching as the primary mechanism of inhibition (bending). On the other hand, recent Direct Numerical Simulations of statistically-planar flames [Nivarti et al. (2017), *Proc. Combust. Inst.*, 36:(in press).] indicate that bending might be achieved in the absence of local quenching. The present study investigates the underlying mechanisms by comparing DNS data with experimental measurements of a lean premixed methane-air flame in high-intensity turbulence.

Girish Nivarti
Department of Engineering,
University of Cambridge
gvn22@cam.ac.uk

Ben Thorne
School of Mechanical Engineering
University of Leeds
mnbjt@cam.ac.uk

Stewart Cant
University of Cambridge
rsc10@cam.ac.uk

Malcolm Lawes, Derek Bradley
School of Mechanical Engineering
University of Leeds
m.lawes@leeds.ac.uk, d.bradley@leeds.ac.uk

CP24

Combustion Simulation of Transportation Package Performance in Severe, Long Duration Fire Using Computational Fluid Dynamics Tools

The Nuclear Waste Management Organization (NWMO) is responsible for the long term management of Canadas used nuclear fuel. Transportation of radioactive material must be carried out in very robust transportation packages. Transportation package robustness is demonstrated by satisfying stringent regulations set by nuclear regulators. The nuclear regulator in Canada, the Canadian Nuclear Safety Commission, adopts regula-tions by the International Atomic Energy Agency. One of many demonstration tests in the regulations subjects a transportation package to an 800C, fully engulfing fire for 30 minutes. That regulatory test bounds conditions in historic transportation fire accidents but its severity is difficult to communicate to the general public; especially in comparison to recent real-world transportation accidents involving severe fires. NWMO is building an advanced computational fluid dynamics combustion model to simulate real-world long duration transportation accident fires. This fire simulation model will help study transporta-tion package performance in hypothetical severe fires. Developing such a model and knowledge will help bridge the information gap between the 30 minute regulatory thermal test and real world long du-ration transportation accident fires. This paper describes the development of NWMOs combustion simulation model in ANSYS Fluent; benchmarking of the model against real-world test data; as well as challenges encountered and les-sons learned.

Yang Sui
Nuclear Waste Management Organization
ysui@nwmo.ca

CP24

Direct Numerical Simulations of Dimethyl-Ether

(DME)/Air Mixture Auto-Ignition with Temperature and Velocity Fluctuations

Direct numerical simulations (DNS) were conducted to investigate the fundamental auto-ignition characteristics of dimethyl-ether (DME)/air mixtures in the presence of velocity and temperature fluctuations. A main scientific objective is to characterize the ignition behavior (regimes) for complex fuels exhibiting non-monotonic ignition delay times with temperature, namely the negative temperature coefficient (NTC) fuels, as the bulk mixture temperature falls in the low, intermediate, and high temperature conditions. The periodic boundary condition is imposed for all boundaries to mimic a constant volume combustion vessel, the Passport-Pouquet kinetic energy spectrum is used to initialize the turbulent velocity field and a similar spectrum method is employed for temperature fluctuations initialization. A reduced 30 species DME oxidation mechanism is used for the chemical production rate calculations. The present study also showcases a first application of the KAUST adaptive reacting flow solver (KARFS) developed for hybrid CPU/GPU computational hardware. Several parametric simulations reveal different ignition behavior ranging from flame propagation to nearly homogeneous ignition. The effect of the intermediate chemistry at the NTC conditions on the ignition characteristics are examined in detail, thereby providing insights into relevant issues in modern internal combustion engine development, such as pre-ignition and knock.

Xiao Xu, Bok Jik Lee
King Abdullah University of Science and Technology
xiao.xu@kaust.edu.sa, bokjik.lee@kaust.edu.sa

Ramanan Sankaran
Center for Computational Sciences
Oak Ridge National Laboratory
sankaranr@ornl.gov

Francisco Perez
Clean Combustion Research Center, King Abdullah University
francisco.hernandezperez.1@kaust.edu.sa

Hong Im
King Abdullah University of Science and Technology
hong.im@kaust.edu.sa

CP25

Numerical Analysis of the Lagrangian Particle Transport of a Confined Stage Can Combustor

The primary purpose of this study is the development of PDF-type of models of the trajectories and deposition of particles from high-fidelity Lagrangian simulation of an industrial Siemens combustor [1,2]. The test case has been previously investigated by the authors [2] and good correlation with the experimental data was obtained at all locations. The motivation comes from the interest in the development of atomization and evaporization models for industrial gas turbines. Eulerian models are cheaper than Lagrangian models, but require the use of subgrid scale models to describe the particle trajectories. The present work is focused on the development of a methodology to obtain PDF models for Eulerian simulations using large-scale Lagrangian simulations in the context of LES. The strategy is based on analysing the fluid particles trajectories and elaborate PDF models that can reproduce the flow behaviour. The emphasis is given to the description of the mixing lines, analysis of flow patterns, particle deposition, Lagrangian trajectories and focus on the development of subgrid scale models and PDF-type of models for this particular configuration. Lagrangian simulations with different number of particles and sizes will be conducted in order to identify the main trajectories and generate PDF-type models that can be used in both RANS and LES.

Daniel Mira
BSC-CNS
daniel.mira@bsc.es

Oriol Lehmkuhl
BSC
oriol.lehmkuhl@bsc.es

Enric I. Mahiques, Lukasz Panek
Siemens
enric.illanamahiques.ext@siemens.com,
lukasz.panek@siemens.com

Mariano Vazquez, Guillaume Houzeaux
BSC
mariano.vazquez@bsc.es, guillaume.houzeaux@bsc.es

CP25

CFD Modeling of Water Mist Suppression of Solid Combustible Fires Using Firefoam

Water-based suppression systems have been frequently used to protect solid combustible products in warehouse occupancies. Understanding the suppression physics can help design an effective fire suppression system. In this study, water mist suppression of rack storage fires of a 2x4 by 2 tier high fuel array is investigated. Water mist spray typically has low water delivery density and small droplets on the order of 0.1 mm. One of the key suppression physics is direct gas-phase flame quenching. The small droplets evaporate quickly in a fire environment and produce a large amount of water vapor. Spray evaporation cools the flame and the generated water vapor dilutes the local oxygen. The high velocity spray also disturbs the flame and increases the flame strain rate. These effects change the energy balance between local heat release rate and heat loss rate, which may lead to local flame extinction. In addition to flame extinction, spray wetting/cooling of the burning surfaces and radiation attenuation can also enhance the spray suppression effectiveness. This study targets modeling fire suppression with the aforementioned suppression physics in a CFD code. Specifically, gas-phase flame extinction is modeled based on the Damkhler number concept and the surface wetting/cooling is modeled with a thin water film flow on solid surfaces. The modeling results are compared against a series of full-scale suppression tests with different nozzle, drop size and pressure.

Ning Ren, Hong-Zeng Yu, Karl Meredith, Ankur Gupta, Yi Wang
FM Global
ning.ren@fmglobal.com, bert.yu@fmglobal.com, karl.meredith@fmglobal.com, ankur.gupta@fmglobal.com, yi.wang@fmglobal.com

CP25

Numerical Investigation and Optimization of Porous Media Burners

Combustion in porous media represents a promising com-

bustion technology for achieving lower emissions, enhanced flame stabilization, and improved fuel efficiency compared to conventional free-flame systems. In these burners, combustion is facilitated inside a porous matrix that is made of a heat-conducting material to enable internal heat-recirculation and achieve super-adiabatic combustion by preheating the unburned reactant mixture to temperatures that sustain chemical reactions. The objective of this study is to computationally examine the stability of combustion in porous media burners (PMBs). To this end, low-order and high-fidelity models are developed to enable the prediction of the heterogeneous combustion and conjugate heat transfer inside the porous structure. Experimental data from X-ray computed tomography, thermocouples, and pressure probes are used for model validation. Following the model validation, parametric studies are performed to examine the stability and emissions of PMBs over a range of operating conditions, including mass flow rates, equivalence ratios, and material properties of the porous matrix. By employing computational optimization of pore size and pore-distribution, a new burner concept is identified that exhibits superior performance properties compared to conventional PMB-designs in terms of pressure drop, emissions, and flame stability. This optimized PMB-design is demonstrated experimentally to validate computational predictions.

Sadaf Sobhani, Danyal Mohaddes
Stanford University
ssobhani@stanford.edu, danmohad@gmail.com

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

CP25

Numerical Simulation on Lean Premixed High Swirl Flame Flashback

In hydrogen-rich fuel based gas turbines, the issue of boundary layer flashback is a key safety concern. Due to the wide flammability range of hydrogen combined with its high reactivity, a premixed flame can propagate along boundary layers. This upstream motion can locate the flame inside the premixing chamber, which is typically not designed for high temperature fluids. Hence, understanding the physics of boundary layer flashback is important for developing designs that arrest such upstream flame motion. In this work a model premixed swirl combustor, experimentally studied at UT Austin, is simulated using large eddy simulation methodology. A novel flame-generated manifold approach is used to capture the flame propagation. Flame flashback is initiated by increasing the inflow equivalence ratio in the experiment. To simulate this effect, a variable equivalence ratio stratified flame model is developed. A flamelet-generated manifold is developed, where each flamelet solution is simulated by accounting for a wall heat-loss parameter. The solution is then mapped to a progress-variable/enthalpy loss space. Different strategies for developing the flamelet tables are discussed in this context. Simulations show that flashback proceeds in the low-velocity streaks found near the wall. Further, flashback circumvents the swirling motion, with the flame jumping across streamlines. This is contrary to methane-air flames, where flashback follows the swirling motion of the fuel-air mixture.

Yihao Tang, Malik Hassanaly
Department of Aerospace Engineering
University of Michigan
yhtang@umich.edu, malik.hassanaly@gmail.com

Venkat Raman
University of Michigan
ramanvr@umich.edu

CP25

Modeling of Light-Round in An Annular Combustor Operating under Perfectly Premixed Conditions

The results from the large-eddy simulation (LES) of light-round in an annular combustor operating under perfectly premixed conditions are analyzed in order to model the flame propagation during the ignition process. In particular, the absolute velocity of the turbulent flame front is a key quantity which controls the duration of the light-round process. It depends on the resolved and subgrid-scale flame wrinkling but also on the gas volumetric expansion. Under the specific configuration of an annular chamber, this expansion is modified during the ignition process by the outflow at the exhaust boundary of variable mass flow rates of fresh and burnt gases. Considering global budgets of species, mass and momentum combined with hypotheses supported by the LES results enables to quantify the coupling of the different phenomena that have been observed and to derive a macroscopic model for the absolute turbulent burning velocity. The range of validity of the model is finally assessed for different operating points.

Maxime Philip, Ronan Vicquelin, Thomas Schmitt
EM2C, CNRS, École Centrale Paris
maxime.philip@ecp.fr, ronan.vicquelin@centralesupelec.fr, thomas.schmitt@ecp.fr

Sébastien Candel
EM2C, CNRS, CentraleSupélec
sebastian.candel@ecp.fr

CP25

Detailed Investigation of the Two-Phase Reacting Flow in An Aeronautical Test Rig

Even if a great effort has been devoted to the predictive modeling and simulation of aeronautical-like configurations in gaseous conditions, two-phase configurations are still challenging to simulate because of the complex interactions between the spray, the flame and the flow field, especially in a Large Eddy Simulation (LES) context. In this work, we focus on the description of the spray phase, by investigating the impact of the polydispersity on the spray flame. To do so, we compare the results obtained from a monodisperse description and from a Multifluid approach. To ensure a correct characterization of the chemistry, we use an analytical chemistry solving for 24 species, expressly developed for dodecane. Investigations are concentrated on the spray and fuel distribution in the combustion chamber, as well as on the spray-flame interactions, in order to highlight the effects of polydispersion.

Aymeric Vié
Laboratoire EM2C
CNRS-CentraleSupélec
aymeric.vie@centralesupelec.fr

Benedetta G. Franzelli
Ecole Centrale Paris, EM2C CNRS UPR-288

benedetta.franzelli@ecp.fr

CP26

Adequate Techniques for the Practical Computation of Optimal Estimators

Modeling unclosed terms in partial differential equations requires to express these terms as a function of known quantities and typically involves two steps: First, a set of known quantities needs to be specified as input parameters for the model, and second, a specific functional form needs to be defined to model the unclosed terms by the input parameters. Both choices involve a certain modeling error, with the former known as the irreducible error. Typically, only the total modeling error is assessed, but the concept of the optimal estimator applied here enables the separate analysis of both the total and the irreducible error. Additionally, it enables the identification of optimal input parameter sets for a certain model by a systematic analysis of irreducible errors. This concept has been applied in the context of a priori analyses of turbulent combustion models as the complexity of DNS necessitates such systematic analysis tools. So far, little attention has been paid to the techniques themselves required for the practical computation of irreducible errors. Particularly for large numbers of input parameters, the choice of technique strongly affects the outcome of the analysis so that, in this work, a comparison among different techniques is presented. Moreover, a strategy for the systematic reduction of irreducible errors is discussed. The findings are applied to modeling the soot intermittency in LES using a DNS data set of a sooting temporally-evolving n-heptane jet.

Lukas Berger
Institute for Combustion Technology
RWTH Aachen University
l.berger@itv.rwth-aachen.de

Heinz Pitsch
Aachen University
h.pitsch@itv.rwth-aachen.de

Michael E. Mueller
Princeton University
muellerm@princeton.edu

CP26

Dynamics of Combustion Systems Using Lyapunov Analysis

Transient processes are an important class of combustion problems relevant to flashback, thermoacoustic instabilities, ignition, relight and blow-off in gas turbines. For such flows, the use of statistical tools is not optimal due to the low frequency occurrence of key events. In order to develop a methodology for understanding low frequency or rare events, a dynamic systems approach is followed here. Such techniques have been widely used for studying low-dimensional chaotic systems in the past. With the increase in computational power, there is a new opportunity to apply such methods to the high-dimensional turbulent combustion problem. As a first step, a characterization of rare-events is provided in terms of this dynamic systems approach. Further, Lyapunov spectrum is computed for canonical turbulent flames to understand the nature of strange attractors for theses systems. A method to obtain rare trajectories by conducting forced simulations is then discussed. Application to flame propagation in homogeneous turbulence is presented.

Malik Hassanaly
Department of Aerospace Engineering
University of Michigan
malik.hassanaly@gmail.com

Venkat Raman
University of Michigan
ramanvr@umich.edu

CP26

Stochastic Modeling of Combustion

A variety of turbulent flows both with and without combustion have considered. Stochastic modeling of turbulent flows is discussed in terms of velocities and compositions. Monte Carlo method and turbulent diffusion flame calculation with thermo-chemical schemes involving upto three composition variables with finite rate kinetics is discussed in this paper.

Salam Khan
Alabama A & M University
salam.khan@aamu.edu

CP26

Characteristics of a Partial Premixed Bluff Body Low NOx Burner

A novel partial premixed bluff body (PPBB) burner has been investigated numerically. The burner features a frustum shaped bluff body that generates a flame stabilizing recirculation zone. Hydrogen is partially premixed in an accelerated air cross-flow before reaching the combustion zone. The burner operates at lean conditions and incorporates internal flue gas recirculation to achieve low NOx emission levels. Experimental investigations have proven good emission-performances at laboratory scale (10 kW). However, the scalability of the burner is not well understood yet. Computational fluid dynamic (CFD) simulations have therefore been conducted to investigate the governing fluid and thermodynamic characteristics of the burner. The numerical model has been validated against experimental data obtained by 2D particle image velocimetry (PIV) measurements for cold and reacting flow conditions. The degree of premixing and the extent of dilution due to recirculation of combustion products have been quantified and different flame regions have been characterized.

Christoph Meraner
Norwegian University of Science and Technology
christoph.meraner@ntnu.no

Mario Ditaranto
SINTEF Energy Research
mario.ditaranto@sintef.no

Terese Lovas
Norwegian University of Science and Technology
terese.lovas@ntnu.no

CP26

A Combination Between Two Semi-Analytical Method Called "Singularly Perturbed Homotopy Analysis Method, (spham)" Applied to Combus-

tion of Spray Fuel Droplets

In our research we combined two well-known analytical methods: the Homotopy Analysis Method (HAM) and the Method of Integral (invariant) Manifold (MIM) to investigate the problems of auto-ignition of a polydisperse fuel spray. We call this combination the Singularly Perturbed Homotopy Analysis Method (SPHAM). In many cases, combustion processes are described by mathematical models that includes a set of highly nonlinear differential equations that are characterized by a different time scale (so-called multi-scale systems). For example, the temperature is a fast variable, due to the Arrhenius factor, compared to the radius evolution variable (the evaporation process). We apply the SPHAM method to problems of thermal explosion in two phase combustible mixtures of gas with polydisperse fuel droplets. We analyze a dependence of our analytical and/or numerical results for different practical probabilistic distributions of fuel droplets, that are modeled by continuous probability distribution functions. By applying the SPHAM, we derived an analytical solution of the system for comparatively simple models of thermal explosion and compared our results with numerical simulations.

Ophir Nave
Hashachar street 24 Beit Hakerem Jerusalem
naveof@cs.bgu.ac.il

CP26

Mode Determination for Combustion Modeling in Partially Premixed Turbulent Flames

The cost of turbulent combustion simulations can be drastically decreased by using reduced-order manifolds (e.g. flamelets) to approximate local thermochemical states. These manifolds are typically generated from one-dimensional flame calculations with boundary conditions appropriate for the global combustion mode of the turbulent flame being simulated. For multimodal turbulent flames, the manifold must include one-dimensional calculations with a range of boundary conditions corresponding to nonpremixed, premixed, and partially premixed flames. The transition between the combustion modes is specified through either a local indicator or the flamelet boundary conditions. In this work, a new flamelet approach for multi-modal combustion is applied in large eddy simulation (LES) of the Sydney jet flame with inhomogeneous inlets. A second mixture fraction is required to characterize the mixing within this three-stream configuration; this provides a suitable parameter to indicate the combustion mode and define the flamelet boundary conditions. Unlike previous mode switching models, this approach intrinsically accounts for both multimodal combustion and the effects of mixture inhomogeneity. It is shown that new approach captures the evolution from largely premixed combustion near the nozzle to nonpremixed-like combustion downstream that is seen experimentally in the Sydney flame.

Bruce A. Perry
Department of Mechanical and Aerospace Engineering
Princeton University
baperry@princeton.edu

Michael E. Mueller
Princeton University
muellerm@princeton.edu

MS1

A Multi-Scale Model of Compaction-Driven Initiation of Detonation

In heterogeneous explosives, sites of high temperature and pressure, called hot spots, play a significant role in detonation initiation. This study seeks to model hot spots generated by the compaction of a granular explosive. Two scales are considered, a macro scale modeled as compressible reactive flow with compaction coupled to a grain scale represented by a reaction-diffusion system. Well-resolved numerical results are presented for initiation and propagation of detonation.

James R. Gambino
Lawerence Livermore National Lab
gambino1@llnl.gov

Donald W. Schwendeman
Rensselaer Polytechnic Institute
Department of Mathematical Sciences
schwed@rpi.edu

Ashwani K. Kapila
Rensselaer Polytechnic Inst.
kapila@rpi.edu

MS1

Whole-System Detonation Modelling for Practical Applications

Contemporary industrial combustion applications often involve the two-way interaction of detonation processes with geometrically complex, several-material structures. In this work we present a mathematical and numerical framework for multi-physics and multi-scale whole-system simulations, where the governing equations for condensed-phase explosives, inert fluids and elastic-plastic solids are solved simultaneously. We focus on applications involving explicit detonator modelling and underground charges simulation for the generation of synthetic seismic data. Each application has its own challenges, depending on the number and type of materials involved and governing lengthscales and timescales.

Eleftherios Ioannou
University of Cambridge
ei233@cam.ac.uk

Louisa Michael
Laboratory for Scientific Computing
University of Cambridge
lm355@cam.ac.uk

Nikolaos Nikiforakis
University of Cambridge
nn10005@cam.ac.uk

MS1

Propagation Limit of Detonation Waves in a Spatially Heterogeneous Reactive Medium with Yielding Confinement

The effect of two-dimensional spatial heterogeneities on the propagation limit of detonation waves governed by single-step Arrhenius kinetics and yielding confinement is com-

putationally examined in this study. The reactive medium consists of a calorically perfect gas. The heterogeneities are implemented via introducing a spatially regular or random variation in the initial concentration of the reactant. In order to investigate the propagation limit, losses due to lateral expansion are realized by placing an inert layer confining the detonable mixture. The deficit in propagation speed from the corresponding Chapman-Jouguet value is expected, as a loss in momentum is experienced by the detonation wave. A critical charge thickness below which a steady propagation cannot be sustained is numerically determined. The resulting detonation speed deficits and critical thicknesses from the simulations for the cases with homogeneous and heterogeneous reactive media are compared with the analytic results obtained using a quasi-one-dimensional, ZND-like model based on the assumption of a smoothly curved detonation wave front. A percolation-like mechanism that assists a detonation wave to propagate beyond the limit that would be encountered in a homogeneous system might be identified in the cases with randomly distributed heterogeneities.

XiaoCheng Mi
McGill University
xiaocheng.mi@mail.mcgill.ca

Andrew Higgins
Department of Mechanical Engineering
McGill University
andrew.higgins@mcgill.ca

Hoi Dick Ng, Charles B. Kiyanda
Concordia University, Montreal, Canada
hoing@encs.concordia.ca, kiyanda@encs.concordia.ca

Nikolaos Nikiforakis
University of Cambridge
nn10005@cam.ac.uk

MS1

Equations of State for Predictive Modelling of Confined, Condensed-Phase Explosives

Modelling of detonation waves requires closure rules for describing the mixing of reactants and products in the reaction zone. Temperature equilibrium, heat isolation and constant volume conditions are among the possible assumptions that can be made. If the temperature equilibrium condition is to be implemented, equations of state capable of producing thermodynamically meaningful values of the temperature are required. To this end, we modify existing equations of state to appropriately approximate the temperature in the reaction zone. Mechanical equations of state of Mie-Gruneisen form are developed with extensions, which allow the temperature to be evaluated appropriately. Furthermore the use of a temperature equilibrium approximation in the context of a hydrocode requires the solution of a non linear equation. The thermodynamically correct asymptotic behaviour of the equations of state that we present ensures this can be solved robustly. We apply the new form of the equations of state in the context of predictive simulation of detonations in compliantly confined rate-sticks.

Simon D. Wilkinson, Nikolaos Nikiforakis
University of Cambridge
sw561@cam.ac.uk, nn10005@cam.ac.uk

Louisa Michael
Laboratory for Scientific Computing
University of Cambridge
lm355@cam.ac.uk

MS2

Open-Source Software for Uncertainty Quantification in Reacting Flows

We present on-going work to provide open-source software tools to enable quantification of uncertainty in reacting flows, including statistical inversion for probability density functions of parameters. We describe the Antioch thermochemistry and transport library that provides an interface to compute kinetic rates, thermodynamics, and transport properties. Antioch also provides an interface for computing solutions to zero-dimensional reactors. We also describe GRINS, a multiphysics finite element framework built on the libMesh finite element library. Within GRINS, we have deployed 1-D, 2-D, and 3-D kernels for the reacting low Mach Navier-Stokes equations suitable for combustion flows. These kernels leverage the Antioch thermochemistry library. We discuss how GRINS and facilitate computations of quantity-of-interest functionals in conjunction with the discrete adjoint problem for enabling adapative mesh refinement and sensitivity calculations. Finally, we describe on-going work to facilitate the interaction between GRINS and the QUESO statistical library for solving statistical inverse problems. Antioch, libMesh, GRINS, and QUESO are all open-source packages, available on GitHub, and are licensed under LGPL 2.1.

Paul Bauman
Mechanical and Aerospace Engineering
University at Buffalo, State University of New York
pbauman@buffalo.edu

MS2

Multifidelity Failure Probability Estimation in Combustion Modeling

The process of robust design of combustion devices often requires computing the probability of failure of the combustion unit. With many uncertain parameters in a combustion model, computing failure probabilities amounts to evaluating the expectation of the failure event, as defined by the engineer. By design, failure probabilities are small, and standard Monte Carlo estimation of the failure integral requires many samples. This gets complicated by the fact that we consider cases where evaluating the QOI requires solving a computationally expensive model, such as a combustion model. We thus propose to use importance sampling to reduce the number of expensive model evaluations. Using a suite of surrogate models, we evaluate the QOI, and design a biasing distribution, that is biased towards failure events. The evaluation of the surrogates is computationally cheap. With this biasing distribution, we can evaluate the original failure proability with much fewer samples - and hence much fewer evaluations of the expensive model - while achieving high accuracy. Numerical examples on a combustion-type test problem illustrate our approach.

Boris Kramer
Massachusetts Institute of Technology
bokramer@mit.edu

Benjamin Peherstorfer
ACDL, Department of Aeronautics & Astronautics
Massachusetts Institute of Technology

pehersto@mit.edu

Karen E. Willcox
Massachusetts Institute of Technology
kwillcox@MIT.EDU

MS2

Towards Model Inadequacy Representations for Flamelet-Based Combustion Models

Flamelet-based models are commonly used to represent combustion in RANS and LES simulations of non-premixed combustion. These models are formulated assuming a separation of scales between the chemistry and the flow, with the chemistry assumed to be fast relative to the turbulence. This allows a turbulent flame to be approximated conceptually as an ensemble of laminar flames. Even when this basic conceptual model is valid, to formulate a practical model, a number of additional modeling choices and approximations are made, including the choice of parameterization of the laminar flame solution, choice of chemical mechanism to generate laminar flame solutions, choice of PDFs characterizing the ensemble, etc. These choices introduce model inadequacy that can lead to inaccurate predictions. In the present talk, we explore the possibility for representing these model inadequacies in the context of a RANS/flamelet model for a turbulent jet flame. It will be shown that the uncertainty in a laminar flame library, due to either chemical parameter uncertainty or chemical model inadequacy, can be effectively represented using a Karhunen-Loève decomposition of the resulting stochastic flame solution. This representation is then exploited to develop a tractable representation of the model inadequacy in the flamelet model.

Todd A. Oliver
PECOS/ICES, The University of Texas at Austin
oliver@ices.utexas.edu

David Sondak
PECOS/ICES, University of Texas at Austin
dsondak@ices.utexas.edu

Chris Simmons
ICES, University of Texas
csim@ices.utexas.edu

Robert D. Moser
University of Texas at Austin
rmoser@ices.utexas.edu

MS2

Calibration of a Stochastic Operator-Based Model Inadequacy Representation for Chemical Kinetics

Two of the most prominent modeling assumptions used in simulations of turbulent combustion are the introduction of turbulence models and reduced chemistry models. In the present work, we develop a stochastic model inadequacy representation to quantify uncertainties due to reduced models in chemical kinetics. The inadequacy formulation is a generalization of previous work in which a stochastic operator is appended to a reduced chemical kinetics model and calibrated with data from a detailed model using a heirarchical Bayesian approach. The inadequacy formulation accounts for situations in which both reactions and species are neglected from the detailed model. The new inadequacy model was developed to be adaptive such that it is only active when chemical reactions are taking place; otherwise the inadequacy model does not participate. We present results from a perfectly stirred reactor of H_2 O_2 combustion. The detailed model consists of 21 reactions and eight species whereas the reduced model uses five reactions and seven species. We then apply the inadequacy formulation to a one-dimensional counterflow diffusion flame with H_2-O_2 combustion. Finally, we present preliminary results on using the counterflow diffusion flame and its associated uncertainties from the inadequacy formulation to build an uncertain flamelet library for non-premixed combustion.

David Sondak
PECOS/ICES, University of Texas at Austin
dsondak@ices.utexas.edu

Todd A. Oliver
PECOS/ICES, The University of Texas at Austin
oliver@ices.utexas.edu

Robert D. Moser
University of Texas at Austin
rmoser@ices.utexas.edu

MS3

Direct Construction of the Steady Traveling High Explosive Cylinder Test

The intent of high explosives (HE) is to perform work on surrounding inert materials. In this respect, it is the HE product equation of state (EOS) that is important. This is indirectly measured through one of several experimental procedures, such as the HE copper cylinder test. In this test, a detonation wave in the HE is allowed to reach steady propagation while driving a copper liner. Often, such experiments are modeled with full time dependent hydrocodes, which results in hours of simulation times on suitable computational meshes. Here, a description of a solution technique to construct the steady traveling wave solution is presented. This may be useful in calibrating HE products EOS as well as for cross-verification of other hydrocodes. The methodology takes advantage of the steadiness of the flow to construct the solution, thus eliminating the independent variable of time. A fast construction can be achieved by marching in a single space dimension. It is convenient to utilize streamline coordinates, as this naturally allows for different EOS for HE and inert materials as well as for allowing material slip. A finite volume methodology allows for discrete conservation of mass, momentum and energy. An approximate Riemann solver based solution technique will be presented. It is shown that solutions can be generated in a matter of seconds at very high resolution, opening up the possibility of rapid calibration of HE products EOS via nonlinear optimization techniques.

Tariq D. Aslam
Los Alamos National Laboratory
Group WX-9, Shock and Detonation Physics
aslam@lanl.gov

MS3

A Thermochemical Algorithm for Combustion Modelling

A new computational tool for predicting the performance of explosives based on chemical composition will be presented. An equation of state for a reacting multi-component, multiphase mixture is constructed by linking a statistical me-

chanics model of high pressure fluids with that of a solid under pressure. The non-linear constrained optimization problem for the thermochemical equilibrium state of the mixture is solved via a sequential quadratic programming method. A novel procedure is incorporated to maintain mechanical equilibrium across phases in the mixture during this process. The resulting thermochemical code is used within the framework of Chapman Jouguet detonation theory to predict the ideal detonation performance of explosives. An extension is presented which aims to capture non-ideal effects by solving a reduced system along streamlines.

Geraint Harcombe, Nikolaos Nikiforakis, Martin Braithwaite
University of Cambridge
gh377@cam.ac.uk, nn10005@cam.ac.uk, mb832@cam.ac.uk

MS3

A New Approach for Cook-Off Modelling

The numerical modelling of slow-initiation or cook-off of explosives has been a subject of great discussion, as the disparate timescales of the heating process and the detonation event generate non-trivial numerical challenges. Cook-off processes involve multiple materials and phases of matter and current numerical simulation methods often rely on coupling different sets of equations to describe them separately. In this work, we adopt a mathematical model able to describe both solids and fluids in a single hyperbolic framework, including a hyperbolic subsystem for thermal conduction, to simulate such processes. A new method is proposed for significantly accelerating the simulation of slow cook-off on short, bounded domains: The acoustic components of the system are approximated by assuming that the pressure roughly equilibrates on a faster time scale than the other processes of the system, and only a reduced subsystem is solved. Examples of applications of the method for cook-off modelling are presented.

Haran Jackson, Nikolaos Nikiforakis
University of Cambridge
hj305@cam.ac.uk, nn10005@cam.ac.uk

MS3

Robust Multi-Dimensional Shock-Fitting

The use of shock-capturing methods in the vicinity of discontinuities typically preclude high rates of convergence of solutions. This suggests that the use of a numerical scheme which fits the shock and material interface can provide a marked improvement on the accuracy of solution. However, such methods often suffer from secondary unfitted discontinuities interacting with the fitted leading shock or material interfaces, *e.g.* triple points or overtaking shocks. In order, to extend the utilization for the recently developed shock and material interface fitting scheme, which is composed of fifth-order spatial and third-temporal discretizations, a switch is added to the algorithm to locally lower the order of the algorithm near the fitted shock when a secondary discontinuity is in the region. This more robust scheme is first applied to an inviscid, detonating, ideal gas propagating in a two-dimensional channel. It is also applied to two-dimensional slab and axisymmetric high-explosive (HE) geometries.

Christopher Romick
Eureka Physics
christopher.romick@gmail.com

Tariq D. Aslam
Los Alamos National Laboratory
Group WX-9, Shock and Detonation Physics
aslam@lanl.gov

MS4

Quantifying Uncertainty from Model Error in Turbulent Combustion Applications

We focus on quantifying the uncertainty associated with model error in large eddy simulations (LES) of a scramjet engine. LES models may involve different parameterizations, and numerical or geometric simplifications in order to achieve computationally tractable simulations, but errors are often introduced from these simplifying physical or numerical assumptions. It is thus imperative to understand and quantify the additional uncertainty induced as a result of using these model alternatives. We introduce a novel strategy for model error quantification by directly embedding a discrepancy representation into the parameters of the models. Armed with higher fidelity simulation data, we then proceed by calibrating both model parameters and discrepancy representation simultaneously. What sets our approach apart is its advantages for accommodating *predictive* engineering applications: the method generates physically meaningful predictions of quantities of interest (QoIs) by automatically respecting the governing equations and physical constraints imposed in the model, and provides an intuitive platform for "extrapolating" the model error for predicting new QoIs. Using a Bayesian perspective, the calibration problem is solved by combining techniques of approximate likelihood, adaptive Markov chain Monte Carlo, and polynomial chaos expansions. Numerical examples comparing static versus dynamic Smagorinsky turbulent models, and 3D versus 2D simulations are presented.

Xun Huan, Khachik Sargsyan, Zachary Vane, Guilhem Lacaze
Sandia National Laboratories
xhuan@sandia.gov, ksargsy@sandia.gov, zvane@sandia.gov, gnlacaz@sandia.gov

Joseph C. Oefelein
Sandia National Laboratories
Combustion Research Facility
oefelei@sandia.gov

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

MS4

Reduced-Order Modeling of Combustion Reactions in Uncertainty Quantification

Abstract not available

Alan Lattimer
Jensen Hughes
alattimer@jensenhughes.com

MS4

Physics-Derived Model Form Uncertainty Quantifi-

cation for Turbulent Combustion

The major challenge in turbulent combustion modeling is the sheer number of models that are invoked, each of which involves its own set of assumptions and subsequent model errors. Quantification of model errors is critical in assessing which model dominates the total uncertainty and should be targeted for future improvements. The fundamental challenge in quantifying model error is in translating model assumptions, inherently coupled to the physics, into mathematical statements of uncertainty. In this work, two methods are presented for deriving model error estimates directly from the physics, bypassing the need for 'training' data, which can never be obtained over all regimes of interest. The first method, peer models, uses models with differing assumptions to derive an uncertainty estimate. This approach will be demonstrated to derive model uncertainty for the scalar dissipation rate time scale. The second method, hierarchical models, uses a higher-fidelity model to estimate the uncertainty in a lower-fidelity model. This approach will be demonstrated to derive model uncertainty for low-dimensional manifold combustion models. The two approaches will be applied to a canonical jet flame configuration to assess the relative contributions of different model errors.

Michael E. Mueller
Princeton University
muellerm@princeton.edu

Venkat Raman
University of Michigan
ramanvr@umich.edu

MS5

Use of Uncertainty Quantification in Tools for Autonomous Scientific Inquiry

Generally, the process of generating kinetic data and improving/validating a kinetic model against data requires time-intensive efforts from computational and experimental researchers. Uncertainty quantification (UQ) of course provides a natural means of automating portions of this process. As examples, UQ-based design of experiments and calculations can identify the most worthwhile data to gather, and inverse UQ can quantitatively improve models based on data. In this regard, UQ, when coupled with automated methods for generating data, provides a means of significantly reducing the amount of time required to gather relevant data and improve/validate kinetic models.

Michael P. Burke
Argonne National Laboratory
mpburke@anl.gov

MS5

Global Sensitivity Analysis with Small Sample Sizes for Large Scale Combustion Simulations

A version of global sensitivity analysis is developed to use for the analysis of complex chemical-kinetic models in combustion devices, such as compression-ignition engines, where typical computations take several processor weeks to complete. It is common in combustion simulations for only a few reactions to have significant sensitivity coefficients and we develop procedures for small-sample size global sensitivity analysis based on this assumption. Because the sample sizes are small and false positives are possible, an important task of this work is calibration, which is done on a chemical model that has been used in engine simulations. This talk will discuss work with several collaborators, in particular: Raghu Sivaramakrishnan, Sibendu Som, Wei Liu, Rex Skodje, and Dingyu Zhou. This work was supported by the U. S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, under Contract No. DE-AC02-06CH11357.

Michael J. Davis
Argonne National Laboratory
Argonne, IL USA
davis@tcg.anl.gov

MS5

Providing Structure to Experimental Data: A Large Scale Heterogeneous Database for Collaborative Model Validation

Experimental data is often stored in various file formats and unfortunately requires highly-specialized codes to parse each individual set of data. The lack of a structured format makes it challenging to find relevant data across a diverse collection for model validation and uncertainty quantification (V/UQ). PrIMes open and flexible data models provide needed structure to experimental data by using the XML file format. Every data value is distinctly labeled, making it simple to search for and make use of data from several sources through a single search query. Recent additions of thousands of coal devolatilization and oxidation experiments highlighted the flexibility of the PrIMe data models, enabling scientists to quickly incorporate validation data from different sources in their V/UQ analysis. A newly developed PrIMe app further allows for easy searching, visualization, and extraction of large amounts of data. We will present a working case utilizing the app along with the coal data warehouse to quickly identify data sets relevant to a specific char oxidation model V/UQ study.

James Oreluk
University of California Berkeley
jim.oreluk@berkeley.edu

MS5

Furnace Design: Extrapolation of Uncertainty

The objective of numerical combustion is to predict combustion quantities of interest in the absence of measured results. The accompanying uncertainty of the model prediction comes from a body of experimental evidence obtained at different scales. The model predictivity is thus an extrapolated (or in some cases interpolated) uncertainty. Traditionally, this extrapolation has been achieved through a hierarchical validation process. The hierarchy is traversed from the bottom up, to obtain the uncertainty for the predicted quantity of interest at the top of the hierarchy. We present a top down uncertainty quantification process that identifies the amount of bias error in all three contributing aspects of the modeling process: model form uncertainty, numerical bias error, and simulation scenario uncertainty. The accuracy required of the modeled quantity of interest is defined by the objectives of the modeling exercise and defines the degree of modeling that is 'good enough'. We demonstrate this process with the design optimization of a new generation ultra-super-critical pulverized-coal fired utility boiler using LES simulations

on 260,000 cores.

Philip J. Smith
University of Utah
Philip.Smith@utah.edu

Sean Smith
The University of Utah
sean.t.smith@utah.edu

MS6

Modeling, Simulation and Validation of an Advanced Oxyfuel Combustor

For the development of new coal combustion technologies advanced methods and tools are needed. In this work experiments and numerical simulations are combined to investigate and understand the underlying physico-chemical processes of coal flames under oxyfuel conditions. A new test-rig is presented bridging the gap between investigations of open gas-assisted lab-scale flames and enclosed self-sustained coal flames. It is designed as a complementary experiment to an existing combustor for self-sustained coal combustion. It retains all important geometrical features of the state-of-the-art coal burner designed for oxyfuel conditions while providing large optical access for detailed spatially and temporally resolved measurements using laser diagnostics. The test-rig is optimized to provide well-defined and well-controlled boundary conditions. To validate and improve existing models the investigation starts with the non-reacting flow and increases complexity stepwise. First large eddy simulations (LES) of the non-reacting flow field are presented together with a quality assessment. The LES results were compared to the flow field measured by stereoscopic particle image velocimetry and residence time distributions captured by concentration measurements of a tracer using laser absorption spectroscopy. The LES methodology captured the flow and residence time distribution in an accurate manner which allows its further extension to reacting conditions.

Samim Doost
FG Energie- und Kraftwerkstechnik
TU Darmstadt
doost@ekt.tu-darmstadt.de

Florian Ries
EKT
TU Darmstadt
ries@ekt.tu-darmstadt.de

Robert Knappstein
FG Energie- und Kraftwerkstechnik
TU Darmstadt
knappstein@ekt.tu-darmstadt.de

Francesca di Mare
Institute for Energy and Powerplant Technology
Darmstadt Uni
dimare@ekt.tu-darmstadt.de

Amsini Sadiki
Department of Energy and Power Plant Technology,TU Darmstadt
sadiki@ekt.tu-darmstadt.de

Johannes Janicka
Institute for Energy and Powerplant Technology
Darmstadt University of Technology, Germany
janicka@ekt.tu-darmstadt.de

Lukas Becker
RSM
TU Darmstadt
becker@rsm.tu-darmstadt.de

Sebastian Bürkle
RSM
TU
brkle@rsm.tu-darmstadt.de

Diego Zabrodiec
Institute of Heat and Mass Transfer
RWTH Aachen University Germany
zabrodiec@wsa.rwth-aachen.de

Steven Wagner
RSM
TU Darmstadt
wagner@rsm.tu-darmstadt.de

Benjamin Boehm
FG Energie- und Kraftwerkstechnik
TU Darmstadt
bboehm@ekt.tu-darmstadt.de

Andreas Dreizler
RSM, TU Darmstadt
dreizler@rsm.tu-darmstadt.de

Reinhold Kneer
Institute of Heat and Mass Transfer
RWTH Aachen University Germany
kneer@wsa.rwth-aachen.de

MS6

Biomass Pyrolysis in a Micro-Fluidized Bed: A Combined Experimental and Modeling Study

Thermochemical conversion of biomass has recently gained a lot of interest as a potential renewable technology to provide both liquid and gaseous fuels from a variety of feedstock, and much progress has been made in advancing both experimental and modeling capabilities. However, efficiently leveraging experimental measurements to validate and subsequently improve numerical simulations of the relevant reactive gas-solid flow systems remains an outstanding challenge, due to the sheer complexity of the conversion process itself, but also due to the lack of best practices in characterizing the reactors operating conditions and post-processing experimental measurements, often qualitative in nature, specifically for comparisons with simulation results. In order to gain direct and practical insight on how to best overcome this challenge, we consider the joint experimental and numerical study of biomass pyrolysis in a micro-fluidized bed reactor (MFBR). Detailed, time-dependent characterization of the gas phase, including permanent gases and some primary tars, is obtained experimentally from GC and single photoionization (SPI) monitoring. Both detailed Lagrange-Euler and simpler one-dimensional approaches are used to simulate the reactor. In this talk, we will discuss practical avenues to exploit the resulting extensive data sets for numerical validation purposes, and the lessons we learned in establishing a valuable feedback loop for model improvement.

Perrine Pepiot, Himanshu Goyal

Cornell University
pp427@cornell.edu, hg345@cornell.edu

Guillain Mauviel, Anthony Dufour, Liangyuan Jia
LRGP
Université de Lorraine
guillain.mauviel@univ-lorraine.fr, anthony.dufour@univ-lorraine.fr, liangyuan.jia@univ-lorraine.fr

MS6

Solid Fuel Jet Flame Experiments and Simulations

Measurements on a combustion field by means of optical diagnostics techniques in addition to conventional contact type measurements have recently become of major interest as tools for validating numerical simulations as well as clarifying the combustion mechanism. In this study, detailed measurements on a pulverized coal combustion coaxial piloted jet flame are conducted to investigate the combustion behavior. The flow field, the particle dispersion and the flame structure, especially the physics in the ignition process, are discussed in detail with the measured data by shadow Doppler particle analyzer (SDPA), multicolor integrated receiving opitcs (MICRO), a two-color radiation pyrometer, OH and PAH planar laser induced fluorescence (OH- and PAH-PLIF), Mie scattering and time-resolved laser induced incandescence (Tire-LII). The effect of pilot flame is also discussed. A large-eddy simulation on this jet flame was also performed to demonstrate the capability of the numerical simulation. The simulation results were assessed with comparison to the measured data in terms of submodels' capability, such as models for devolatilization, char combustion and gaseous phase reactions. Finally, a strategy of further model validation for a pulverized coal combustion from the experiment is discussed.

Hiroaki Watanabe
Department of Mechanical Engineering
Kyushu University
whiroaki@mech.kyushu-u.ac.jp

Kazuki Tainaka
Energy Engineering Research Laboratory
Central Research Institute of Electric Power Industry
CRIEPI
tainaka@criepi.denken.or.jp

MS6

1-D Flame Configuration for Validating Pulverized Coal Devolatilization and Oxidation Modeling

Joined experimental and numerical studies of devolatilization and oxidation of pulverized coal particles are conducted. The target configuration is a laminar axisymmetric methane/air strained-flow burner fed by coal particles. The flame is impinging a wall surface to enhance stabilization. Coal particles reactions take place in the hot region of the methane/air mixture. Visualization of OH*, CH* and C2* chemiluminescence, Laser Induced Fluorescence measurements of OH radical and flame emission spectroscopy are performed to identify the chemical flame structure and species concentration. The inlet fresh gas boundary conditions are well characterized in the experiments in terms of gas velocity but also number of coal particles and mean particle diameter. Numerical investigations are performed, where the governing equations are fully coupled between gas and particle phase. Detailed kinetic mechanisms, NOx chemistry and OH*/CH*/C2* sub-mechanisms are considered for gas-phase kinetics. Coal devolatilization submodels are challenged on this configuration for describing particle conversion. The analysis of obtained results confirm that the presence of heavier hydrocarbons released by coal pyrolysis has a significant influence on the CH* and C2* concentration in the post-flame region. Finally, the effects of volatile matter composition, strain rate and particle size on pollutant formation are studied.

Meng Xia
EM2C laboratory, CentraleSupelec
meng.xia@centralesupelec.fr

Philippe Scouflaire
Laboratoire EM2C, Centrale Supélec
philippe.scouflaire@centralesupelec.fr

Benoit Fiorina
Laboratoire EM2C, Ecole Centrale Paris
benoit.fiorina@centralesupelec.fr

Nasser Darabiha
Laboratoire EM2C
CNRS-CentraleSupélec
nasser.darabiha@centralesupelec.fr

MS7

Chemical Model Reduction Under Uncertainty

We outline a strategy for chemical kinetic model reduction under uncertainty. We present highlights of our existing deterministic model reduction strategy, and describe the extension of the formulation to include parametric uncertainty in the detailed mechanism. We discuss the utility of this construction, as applied to hydrocarbon fuel-air kinetics, and the associated use of probabilistic error measures between predictions from detailed and simplified models.

Habib N. Najm
Sandia National Laboratories
Livermore, CA, USA
hnnajm@sandia.gov

Mauro Valorani
Dept. Meccanica e Aeronautica
Univ. Rome La Sapienza
mauro.valorani@uniroma1.it

Riccardo Malpica Galassi
Dept. of Mechanical and Aerospace Engineering
Univ. Rome La Sapienza
riccardo.malpicagalassi@uniroma1.it

MS7

Quantifying Variability in Sub-Models for LES of Reacting Flows

The multiphysics, multiscale nature of turbulent reacting flows makes these systems one of the most challenging to understand. Highly nonlinear fluid dynamic, thermodynamic, transport, chemical, and multiphase processes are intrinsically coupled and must be considered simultaneously to satisfy the governing equations. The nonlinear nature of the system limits the number of assumptions that can be made without introducing significant errors. Conversely, significant assumptions must be made to derive multiscale closures that are both accurate and affordable. To find an optimal balance, variability of individual sub-models and their coupled performance must be quan-

tified. In the current work, progress toward this goal is presented in the context of Large Eddy Simulation (LES). Emphasis is on treatment of direct injection processes at Diesel engine conditions using the Sandia n-dodecane-air experiments for validation. The extreme variability between leading chemical mechanisms is highlighted. This variability is accounted for using a novel model mechanism optimized to reproduce autoignition delay times to within a specified tolerance. This is accomplished using Bayesian inference with a model-error representation. Error bars on the predictions are obtained by quantifying the impact of parameter uncertainties. Results are validated using experimental data, then analyzed to gain further insights on potential sources of error and variability in the flow.

Joseph C. Oefelein
Sandia National Laboratories
Combustion Research Facility
oefelei@sandia.gov

Guilhem Lacaze, Layal Hakim
Sandia National Laboratories
gnlacaz@sandia.gov, lhakim@sandia.gov

MS7

Black Swans, Dragon Kings and the Science of Rare Events in Turbulent Combustion

The focus here is on anomalous behavior of systems under otherwise nominal operating conditions. Such events occur due to the indeterminacy of a complex chaotic system given a set of macroscopic operating parameters. Here, we propose a dynamical systems approach to studying rare events. In particular, we are interested in the formalism that allows for such events to be simulated. This talk will cover the classification of rare events, and provide preliminary analysis using canonical configurations. The computational tools necessary for such risk prediction will be discussed in the context of propagation algorithms used for uncertainty quantification.

Venkat Raman
University of Michigan
ramanvr@umich.edu

Malik Hassanaly
Department of Aerospace Engineering
University of Michigan
malik.hassanaly@gmail.com

MS7

Development of An UQ-Predictive Chemical Reaction Model for Syngas Combustion

An automated data-centric infrastructure, Process Informatics Model (PrIMe), was applied for validation and optimization of a syngas combustion model. The Bound-to-Bound Data Collaboration (B2B-DC) module of PrIMe was employed to discover the limits of parameter modifications based on the systematic uncertainty and consistency analysis of the model-data system, with experimental data including shock-tube ignition delay times and laminar flame speeds. The initial H2/CO reaction model, assembled from 73 reactions and 17 species, was subjected to a B2B-DC analysis. For this purpose, a dataset was constructed that included a total of 167 experimental targets and 55 active model parameters. Consistency analysis of the composed dataset revealed disagreement between models and data. Further analysis suggested that removing 45 experimental targets, 8 of which were self-inconsistent, would lead to a consistent dataset. This dataset was subjected to a correlation analysis, which highlights possible directions for parameter modification and model improvement. Additionally, several methods of parameter optimization were applied, some of them unique to the B2B-DC framework. The optimized models demonstrated improved agreement with experiment, as compared to the initially-assembled model, and their predictions for experiments not included in the initial dataset (i.e. a blind prediction) were investigated.

Nadja Slavinskaya
DLR Stuttgart Germany
nadja.slavinskaya@dlr.de

Mehdi Abbasi
German Aerospace Center(DLR), Institute of Combustion Tech.
70569, Stuttgart, Germany
mehdi.abbasi@dir.de

Jan Hendrik Starcke, Aziza Mirzayeva
German Aerospace Center (DLR), Institute of Combustion Tech
70569, Stuttgart, Germany
janhendrik.starcke@dlr.de, aziza.mirzayeva@dlr.de

Wenyu Li, James Oreluk, Arun Hegde
University of California Berkeley
wenyuli@berkeley.edu, jim.oreluk@berkeley.edu, arun.hegde@berkeley.edu

Andrew Packard
U of California at Berkeley
apackard@berkeley.edu

Michael Frenklach
University of California at Berkeley
myf@me.berkeley.edu

G. Gerasimov, O Shatalov
Institute of Mechanics, M. V. Lomonosov Moscow State U
1 prosp. Michurinskii, Moscow, 119192, Russia
gerasimov@imec.msu.ru, shatalov@imec.msu.ru

MS8

Dns of Turbulent Lean Methane-Air Piloted Jet Flames at High Karlovitz Number

DNS of a high Karlovitz number lean methane/air piloted premixed round jet flame is performed to understand the flame structure and propagation response to intense shear-driven turbulence. A reduced chemical model is incorporated in the DNS with 28 species based on GRI-Mech 3.0 including NO chemistry. The flame is in the broken-reaction zones regime and the preheat, inner reaction and oxidation layers are affected by turbulent strain and mixing. In the present study a multi-scale decomposition of turbulent stretch rate and scalar dissipation rate will be presented highlighting the effects of large- and small-scale turbulent mixing and stretch on the flame structure and wrinkling. Multi-scale statistics will be presented at different locations in the flame brush and at different axial locations in the jet.

Haiou Wang
University New South Wales
haiou.wang@unsw.edu.au

Evatt R. Hawkes
University of New South Wales
evatt.hawkes@unsw.edu.au

Jacqueline Chen
Combustion Research Facility
Sandia National Laboratories
jhchen@sandia.gov

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

MS8

Turbulence-Flame Interactions in High-Speed Premixed Reacting Flows

The interaction between a premixed flame and the turbulence in which it propagates is a fundamental problem in combustion theory. The ability to describe these interactions both qualitatively and quantitatively is required for practical problems ranging from the design of clean and efficient combustion engines to the development of next-generation scramjet propulsion. Turbulence-flame interactions are also central to astrophysical problems, such as explosions of type Ia supernovae. In all of these contexts, turbulent fluid velocities can be large such that fluid mixing, even at the scale of the flame, is substantially larger than characteristic heat release or chemical time scales, resulting in Karlovitz (Ka) numbers of order 10^2 or more. For such high Ka reacting flows, there can be substantial changes to the flame structure and burning rate. In this talk, we use direct numerical simulations (DNS) to explore these changes for different values of Ka and for different fuels. Changes in flame structure, burning rate, and chemical species evolutions are examined using both Eulerian and Lagrangian analysis approaches, and the effects of premixed flames on the dynamics of the vorticity, turbulence intermittency, and kinetic energy spectral dynamics are presented. The implications of these results for modeling of turbulent combustion are discussed.

Peter Hamlington
University of Colorado, Boulder
peter.hamlington@colorado.edu

Alexei Poludnenko
Texas A&M University
apoludn@tamu.edu

MS8

Distributions of Flow Topology and Enstrophy in Different Turbulent Premixed Combustion Regimes: A Direct Numerical Simulation Investigation

Three-dimensional direct numerical simulation (DNS) data containing freely propagating statistically planar H2-air flames at three different Karlovitz number conditions were analysed in order to investigate the distribution of flow topologies at different turbulent premixed combustion regimes. The flow topologies were characterized in terms of three invariants of velocity gradient tensor, namely P, Q and R, representing the negative of dilatation rate, strain rate, and enstrophy, respectively. The flow topologies were further categorized in eight types, i.e. S1-S8, depending on the location of velocity gradient tensor in P-Q-R space. It was found that the weakening of dilatation rate with increasing Karlovitz number plays a key role in flow topology and enstrophy distribution in turbulent premixed flames. The contributions to enstrophy transport conditional on topology were analysed in detail and it was found that the enstrophy generation mechanism due to the baroclinic torque weakens as the conditions move from the corrugated flamelets to the broken reaction zone regime.

Hong G. Im
King Abdullah University of Science and Technology
hong.im@kaust.edu.sa

Bill Papapostolou, Daniel Wacks
Newcastle University
nilanjan.chakraborty@newcastle.ac.uk,
nilanjan.chakraborty@newcastle.ac.uk

Markus Klein
Technische Universitaet Darmstadt
Institut fuer Energie und Kraftwerkstechnik, Germany
kleinm@hrzpub.tu-darmstadt.de

Nilanjan Chakraborty
Newcastle University
nilanjan.chakraborty@newcastle.ac.uk

MS8

High Karlovitz Turbulent Flames: Is-This Only a Laboratory/DNS Toy Problem?

High Karlovitz number flames have been discussed at many places in the literature in the context of Borghi regime diagrams. Along these lines, the amplitude of the Karlovitz numbers expected in various combustion systems is first discussed. Then, the regime of high Karlovitz premixed and non-premixed piloted flames is investigated using micro-mixing modelling coupled with complex chemistry. From the results, it is attempted to calibrate the flux of energy flowing from the burnt gases to the reaction zones in order to maintain high Karlovitz combustion. Conclusions are drawn concerning the generic character of such flames.

Luc Vervisch
INSA Rouen CNRS CORIA
vervisch@coria.fr

MS9

Sparse Resolutions to Inconsistent Datasets Via L1-Minimization

Bound-to-Bound Data Collaboration (B2BDC) provides a natural framework for addressing both forward and inverse uncertainty quantification problems. In this approach, parameter-to-QOI (quantity of interest) models are constrained by experimental observations with interval uncertainty. A collection of such models and observations is termed a dataset and carves out a feasible region in the parameter space, which is representative of the current state of knowledge. Consistency analysis, a key attribute of B2BDC, seeks to characterize this feasible set. If a dataset has a nonempty feasible set, it is consistent. In real-world application, however, it is often the case that collections of experiments and observations are inconsistent. Revealing the source of this inconsistency, i.e., identifying which models and/or observations are problematic, is essential before a dataset can be used for further analysis, such as prediction and optimization. In this presentation, we introduce a constraint relaxation-based approach, entitled the vector

consistency measure, for investigating datasets with numerous sources of inconsistency. This new measure seeks a sparse set of relaxations by minimizing an L1-penalty. The benefits of vector consistency over previous methods of consistency analysis are demonstrated in two realistic gas combustion examples.

Arun Hegde
University of California Berkeley
arun.hegde@berkeley.edu

MS9

Uncertainties in Theoretical Chemical Kinetics

Theoretical chemical kinetics is increasingly being relied on to provide input data for combustion modeling. As a result, an improved understanding of their uncertainty is of increasing importance. Proper descriptions of the uncertainty in theoretical predictions are plagued by various factors including (i) correlations in the errors across the components of the theoretical calculations, (ii) uncertainties in the reference data used to evaluate them, (iii) correlations across different theoretical methods, and (iv) a poor understanding of the uncertainties of some components of the calculation. We will explore these issues through illustrative comparisons of theoretical calculations of enthalpies and thermal rate constants with experimental data and with other theoretical calculations.

Stephen Klippenstein
Argonne National Laboratory
sjk@anl.gov

MS9

Uniform Sampling of Feasible Set: A Hybrid Statistical-Deterministic Method of Uncertainty Quantification

Uncertainty quantification is key to developing predictive and reliable combustion models. The Bound-to-Bound Data Collaboration (B2BDC) framework defines a feasible set of model parameters by constraining models with experimental data. Posterior uncertainty information can be explored by statistical analysis of the feasible set. This presentation extends the B2BDC framework by adding the ability to generate uniform samples of the feasible set. Two rejection sampling methods were investigated with both toy and realistic combustion datasets (GRI-Mech and DLR-SynG). We additionally developed two heuristic methods for high-dimensional problems. The efficiency-accuracy trade-off was compared numerically. Posterior correlations of GRI-Mech and DLR-SynG datasets were observed and will be discussed and interpreted.

Wenyu Li
University of California Berkeley
wenyuli@berkeley.edu

MS9

Automatic Chemical Mechanism Generation using Optimized Rate Rules

Branched alkane species are essential constituents in petroleum transportation fuels. A deep understanding of their oxidation performance contributes to efficient fuel consumption and reduced pollutant formation in combustion devices. However, this becomes possible only after the successful generation of accurate chemical kinetic models. While the majority of available models still needs refinement, new chemical schemes are still missing for a large number of important fuels. A rapid and systematic development of accurate chemical mechanisms for branched alkanes is thus of great interest. Recent studies have shown that consistently updating thermochemistry and reaction pathways while optimizing rate rules for a set of C7-C11 normal alkanes can be further applied to develop accurate chemical kinetic models for larger n-alkanes. This strategy, and its prior knowledge, are adopted in the present study and further extended to develop optimized rate rules for branched alkanes. The approach is also combined with an automatic model development method to facilitate rapid generation of accurate chemical models for larger normal and branched alkanes without specific tuning of rate parameters. It is shown that the models developed using this streamlined approach show very good agreement with experimental data.

Heinz Pitsch
Aachen University
h.pitsch@itv.rwth-aachen.de

Liming Cai
Institute for Combustion Technology, RWTH Aachen University
lcai@itv.rwth-aachen.de

MS10

Controlling Parameters in High Karlovitz Number Flames: Small Scales, Large Scales, and Universality

Turbulent premixed flames are characterized by numerous non-dimensional numbers, including Reynolds, Karlovitz, and Damkhler numbers. Their respective impact on the two-way coupling between turbulence and chemistry has been the subject of several studies already. In this presentation, we will review past results and analyze recent results from Direct Numerical Simulations of various hydrocarbon/air flames. The analysis follows two directions. The first direction focuses on the characterization of the reaction zone surface (in terms of curvature, surface area...) and the evolution of the chemical source terms on that surface. The second focuses on the transformation of turbulence across the flame and is investigated by considering vorticity, its production, its dissipation, and its (an)isotropy. All results confirm that (for a given fuel/air mixture) the Karlovitz number controls entirely the small scale chemical processes, not only the mean and the variance, but also the full distribution of source term fluctuations. This conclusion remains valid regardless of the integral length scale (equivalently the Reynolds number). The evolution of the enstrophy is also strongly influenced by the Karlovitz number; yet, a small dependence on the Reynolds number is observed. This is attributed to the lack of universal behavior in finite Reynolds number flows.

Guillaume Blanquart
California Institute of Technology
g.blanquart@caltech.edu

MS10

Low-Temperature Chemistry in Turbulent Premixed Dodecane Flames

Turbulent lean premixed dodecane-air flames are simulated in a doubly-periodic domain using detailed kinetics and transport with a very recent kinetics model that features

improved descriptions of low-temperature chemistry. In particular, compared with previously published models, the new model shows dramatic shifts in the pyrolysis of the heavy fuel molecules occurring upstream of the primary heat release zone. We explore the impact that turbulent mixing can play before it dissipates through the heat release zone. For realistic values of Karlovitz and Damkohler number, we quantify the effects of the improved chemistry model with respect to earlier models.

Marc Day
Lawrence Berleley National Laboratories
MSDay@lbl.gov

Andrew Aspden
LBNL
AJAspden@lbl.gov

John B. Bell
CCSE
Lawrence Berkeley Laboratory
jbbell@lbl.gov

MS10

Transition of Combustion Mode During Flame-Flame Interaction and its Modeling Implication

Thermochemical conditions in various combustion devices will tend to be leaner, well-mixed, more diluted and distributed using unconventional fuels. Such "green" combustion technologies include syngas or biogas, ultra-lean, diluted and preheated combustion. Combustion of multi-component fuels produces thermo-diffusive instabilities, which increases local flame curvatures and surface area. Propagating flames under ultra-lean and/or diluted conditions have larger flame thickness and smaller flame speed compared to a corresponding non-diluted stoichiometric flame, which yields small Damkohler and large Karlovitz numbers, enhancing convolution of flame surface. Flame–flame interactions are caused as a result of unsteady combustion process, and the occurrence becomes frequent when flame surface fluctuation becomes relatively high for the reasons mentioned above. Several previous studies have investigated flame–flame interactions in the context of formation of fresh reactants pockets. The heat release fluctuation resulted from the pocket formation is reportedly a source of combustion noise, and also could be important for prediction of pollutant formation. Thus, the underlying physics of flame interaction process needs to be understood for numerical modelling and to avoid these adverse effects when employing such combustion technologies.

Yuki Minamoto
Tokyo Institute of Technology
yminamot@navier.mes.titech.ac.jp

MS10

A Priori and a Posteriori Study of a High Karlovitz Number Premixed Turbulent Jet Configuration

In this work, a data set of a Direct Numerical Simulation (DNS) of a turbulent CH_4/air lean premixed jet flame configuration with high Karlovitz number (Ka = 250, based on jet exit conditions) and detailed chemistry is studied. At these conditions, strong turbulence-chemistry interactions lead to large deviations from unperturbed combustion and conventional flamelet based combustion models tend to fail. In an a priori analysis the optimal estimator concept, which allows for an error decomposition, is applied to quantify errors of flamelet based combustion models. Furthermore, this concept is applied to identify the quantities, which optimally parameterize interactions between turbulence and chemistry. These parameters are integrated into a priori formulations of flamelet combustion models to demonstrate the possible improvements of flamelet based models in highly turbulent combustion regimes. Furthermore, a posteriori analysis of this configuration is performed using Large-Eddy Simulations (LES) with two flamelet based combustion models. One is based solely on unstretched flamelet solutions, whereas the other considers strained flamelet solutions. The latter shows improved agreement with the reference data from DNS and experiment. The LES results and its errors are analyzed with regard to further improvement of the flamelet based models.

Konstantin Kleinheinz
Institute for Combustion Technology
RWTH Aachen University
k.kleinheinz@itv.rwth-aachen.de

L. Berger
Aachen University
h.pitsch@itv.rwth-aachen.de

Antonio Attili
RWTH Aachen University, Germany
a.attili@itv.rwth-aachen.de

Haiou Wang
University New South Wales
haiou.wang@unsw.edu.au

Evatt R. Hawkes
University of New South Wales
evatt.hawkes@unsw.edu.au

Heinz Pitsch
Aachen University
h.pitsch@itv.rwth-aachen.de

MS11

Prevention and Promotion of Flame Acceleration and Deflagration-to-Detonation Transition

Physical mechanisms of premixed flame acceleration (FA) due to (i) a finger shape, (ii) wall friction and (iii) in-built obstacles are systematically investigated and compared in the configurations of obstructed and unobstructed combustion tubes (CT). Specifically, the effects of mechanistic and thermal boundary conditions on FA; their interlay with thermal-chemical flame properties; and the possibility to trigger a deflagration-to-detonation transition (DDT) event are quantified. The mechanistic conditions include slip or non-slip walls, smooth or obstructed. The thermal conditions include adiabatic or isothermal (cold or preheated) walls. The thermal-chemical properties are coupled to the onset of the combustion instabilities. Namely, the Darrieus-Landau (DL) and diffusional-thermal (DT) instability modes are mainly described by the thermal expansion factor and the Lewis number Le, respectively. It is shown that adiabatic walls and non-slip walls promote FA, which attains the exponential trend, and the effect is especially strong in the case of obstructed CT. The same impact is provided by higher thermal expansions and for lean non-equidiffusive flames. In contrast, rich non-equidiffusive flames propagate slower, as well as that with cold or preheated walls, where the exponential acceleration trend is

replaced by a liner one or even flame extinction. Based on the combination of these effects, the promotive and preventing strategies for FA and DDT are provided.

V'yacheslav Akkerman
Department of Mechanical and Aerospace Engineering
West Virginia University
Vyacheslav.Akkerman@mail.wvu.edu

Orlando Ugarte
Department of Aerospace Engineering, University of Maryland
College Park, MD 20742, USA
ougartea@mix.wvu.edu

Serdar Bilgili
West Virginia University
sabilgili@mix.wvu.edu

Damir M. Valiev
Combustion Research Facility
Sandia National Laboratories
damir.valiev@umu.se

MS11

Formation and Structure of Accelerating Combustion Wave

In the recent decades theoretical understanding of combustion phenomena, computational power and efficiency of numerical algorithms have grown tremendously. However, the long standing problem of Deflagration-to-Detonation Transition (DDT) is still beyond of quantitative predictions even if modern physical models and numerical integration packages are used. Typically, in studies of the problem of DDT an initial stage of the flame acceleration is somehow absent and typically neglected from consideration. The present talk aims to fill the gap and discusses this stage of the DDT. The study is motivated by recent experimental evidences of so-called shockless transition to detonation observed in an obstructed channel where a flame propagates from an open end to the closed one. The frame of 1D flat deflagration of the hydrogen/oxygen and hydrogen/air systems is employed. We use a very complex model of chemical kinetics and detailed descriptions of molecular diffusion for multi-component mixtures at elevated and variable pressure. In spite of 1D formulation it makes the problem of the flame acceleration a very challenging and demanding for numerical treatments task. In the suggested talk experimental evidences and results of numerical experiments will be represented and discussed.

Viatcheslav Bykov, Andrey koksharov
Karlsruhe Institute of Technology (KIT)
viatcheslav.bykov@kit.edu, andrey.koksharov@kit.edu

MS11

Turbulence Effects on Detonation Propagation and Structure

Comparative studies of turbulent inflow vertical and entropic forcing effects on the three dimensional detonation propagation are conducted via direct numerical simulations based on Navier-Stokes equations and global one-step chemical reaction model. The turbulent vertical and entropic forcing effects on the three dimensional detonation wave structures and front dynamics are analyzed, as well as the detonation effects on turbulent vortex structures. The turbulence field imposed has created small scale wrinkles embedded in the detonation front, apart from the large scale features of detonation without turbulence. The detonation propagating velocity varies from 0.8 to 1.6 CJ velocity and its pdf skewes to sub-CJ velocity and peaks at about 0.9. The detonation velocity recorded with time always preferentially decays, with very rapid accelerations through triple point interactions. Its pdf also skews to sub-CJ velocity, while its overall shape agrees well with V-3. The reaction zone is greatly influenced by the vortex, much more irregular and turbulent and elongated for the turbulent cases. Distributed burning pockets are more likely to be found there. The turbulent kinetic energy is amplified across the detonation, and periodically oscillate downstream the detonation due to the periodically collision of the triple points. Finally, the Favre averaged mean structure of the detonation waves and comparisons with the analytical ZND structure are discussed in detail.

Kun Luo, Tai Jin, Jianren Fan
Zhejiang University
zjulk@zju.edu.cn, jintai@zju.edu.cn, fanjr@zju.edu.cn

MS11

Flame Acceleration in Long Narrow Channels Enhanced by Compressibility Effects

The effects of gas compressibility on the propagation of premixed flames in narrow channels closed at their ignition end have been studied, under adiabatic conditions and in the presence of controlled heat losses. Earlier work has shown that, in sufficiently long adiabatic channels, the flame evolves into a steadily propagating compression-driven flame. The propagation speed of these flames depends exponentially on the constant-volume equilibrium temperature, and is therefore significantly larger than ordinary isobaric flames. In the present work, we show that heat losses control the transition between the slow isobaric and the fast compression-driven flames.

Vadim Kurdyumov
CIEMAT, Madrid
vadim.k@ciemat.es

Moshe Matalon
Univesity of Illinois at Urbana-Champaign
matalon@illinois.edu

MS12

Interfacial and Bulk Thermodynamics in Supercritical Combustion

The thermodynamics of high pressure mixing and combustion are still not well understood. While the change of jet disintegration from liquid jet break-up to a turbulent mixing process at supercritical pressures is well documented, the state of knowledge about the thermodynamic structure of non-premixed flames at supercritical pressure is still incomplete. Previous studies have mainly focused on the phase behavior of inert hydrogen - oxygen mixtures. However, in 1D and LES studies of non-premixed flames, we did not observe such large scale inert real fluid mixing. Instead, under rocket engine conditions, an attached flame separates fuel and oxidizer; the cryogenic oxygen stream undergoes a supercritical liquid to real gas transition - pseudoboiling - before mixing with reaction products. Only traces of water (Y¡0.03) are present in the cryogenic oxygen stream before the mixture transitions to an ideal gas state. While state-of-the-art real fluid CFD mixing rules

based on the extended corresponding states principle predict a single phase flow, vapor-liquid-equilibrium calculations instead show that the water will condense as it diffuses towards the oxygen, even when the oxygen injection temperature is raised to 300 K. As the opening talk of the mini-symposium, we will provide links to the following presentations by emphasizing certain aspects of supercritical combustion modeling, such as the steep density gradients, phase separation, and supercritical fluid properties.

Daniel Banuti
Stanford University
Center for Turbulence Research
dbanuti@stanford.edu

Peter C. Ma, Muralikrishna Raju
Stanford University
peterma@stanford.edu, mraju@stanford.edu

Matthias Ihme
University of Michigan
Mechanical Engineering
mihme@stanford.edu

MS12

Thermodynamic, Dynamic and Structural Properties of Compressed Liquids and Supercritical Fluids

While scientists have a good theoretical understanding of the heat capacity of both solids and gases, a general theory of the heat capacity of liquids has always remained elusive. I will introduce a phonon-based approach to liquids and supercritical fluids to describe its thermodynamics in terms of sound propagation. I will show that the internal liquid energy has a transverse sound propagation gaps and explain their evolution with temperature variations on the P-T diagram. As a result, the experimental evidence for the new thermodynamic boundary in the supercritical state (the Frenkel line) on the P-T phase diagram will be demonstrated. Then, I will report on inelastic X-ray scattering and diffraction experiments combined with the molecular dynamics simulations on supercritical Ar. The presented results unveil the mechanism and regimes of sound propagation in supercritical fluids providing a compelling evidence for the adiabatic-to-isothermal longitudinal sound propagation transition. As a result, a universal link will be demonstrated between the positive sound dispersion phenomenon and the origin of transverse sound propagation revealing the viscous-to-elastic crossover. Both can be considered as a universal fingerprint of the dynamic response of a liquid. They can be used then for a signal detection and analysis of a dynamic response in deep water and other fluids which are relevant for describing their thermodynamics. The consequences of this finding will be discussed.

Dima Bolmatov
Brookhaven National Laboratory
d.bolmatov@gmail.com

MS12

Analytical / Computational Approach to Liquid Injection at Supercritical Pressures

Our findings from three areas of background research will define an approach to the study of liquid injection into gases at supercritical pressure: vaporizing droplets at supercritical pressure, vorticity dynamics of incompressible liquid jets flowing into gas, and supercritical combustion in simple configurations, e.g., counterflow. It will be shown that vorticity dynamics analysis is essential to explain the physical mechanisms; surface dynamics alone tells little. Liquid-jet atomization is the result of a transitional turbulence where, in sequence, smaller and smaller scales are formed driven by the behavior of hairpin vortices. At the cascade end, capillary action forms droplets. Several different cascade processes are identifiable depending on the Reynolds and Weber numbers and the density ratio between the liquid and the ambient gas. Even if one phase exists in extreme cases, these hairpin-vortices mechanisms will be controlling in forming discrete blobs of the injected material. The a priori conclusion that one phase exists at supercritical pressure is based on false lore and not physical law. The question about the phases must be left open until the analysis reaches a conclusion; a proper approach will be defined. Proper equations of state for density and enthalpy and the determination of phase equilibrium, liquid composition due to dissolved gas, energy of vaporization, surface tension, and transport properties for high pressures will be discussed.

William Sirignano
University of California, Irvine
sirignan@uci.edu

MS12

Modeling of High Pressure Sprays and Combustion Based on Phase Equilibrium and Jet Theory with Thermal Radiation

A new CFD spray model has been developed for IC engine simulations that is based on the assumption of local phase equilibrium and jet theory. Phase equilibrium is determined by an advanced solver that is based on rigorous thermodynamics with Peng-Robinson Equation of State. Jet theory is applied for the sub-grid mixing-controlled process and particle-gas momentum exchange, to relax the model grid dependency. The model provides good predictions of spray mixture preparation, and the combustion process is accurately predicted without the need to resolve the jet breakup process. Thermal radiation is also included in the modeling. The influence of radiation on steady state flame temperature and soot formation for the ECN Spray A was studied and was found to be negligible. In this case the contribution of soot to total thermal radiation is small due to its relatively small amount and low temperature, compared to the absorbing gas. However, engine simulations show that thermal radiation can have a significant impact on transient soot formation, and non-linear effects are found for post-injection cases.

Zongyu Yue
University of Wisconsin - Madison
zongyuyue@gmail.com

Rolf Reitz
University of Wisconsin-Madison
reitz@wisc.edu

MS13

Analytical and Computational Description of a Coalmine Fire Scenario

Every year, worldwide, explosive accidents claim numerous lives of workers and customers in industries dealing with combustible gases, dust and other explosive materials. Among these industries, historically, coalmining has one of the highest fatality and injury rates. To reduce the risk of explosions in coalmines, a fundamental physi-

cal understanding of the coal dust / methane / air combustion processes is critically needed. The present work, combining comprehensive analytical endeavors and computational simulations, is a step in this direction. First, to reveal the inner mechanisms of a combustion accident in a coalmine, the key stages and characteristics of premixed flame evolution in a mining passage such as the propagation speeds, acceleration rates and run-up distances are scrutinized, through the analytical studies, in large-scale mining passages. The study is mainly focused on the flame acceleration scenarios due to a finger flame shape and wall friction. It is for the first time that the spatial distributions of the combustion characteristics such as the unstretched laminar burning velocity are incorporated in the analysis. Subsequently, the formulations are revisited by incorporating the effect of compressibility. Additionally, a computational platform is developed to validate the analytical predictions and model the nonhomogeneous distribution of coal dust particles in coalmining passages.

Sinan Demir
West Virginia University
sidemir@mix.wvu.edu

Hayri Sezer, Ali S. Rangwala
Worcester Polytechnic Institute
hsezer@wpi.edu, rangwala@wpi.edu

V'yacheslav Akkerman
Department of Mechanical and Aerospace Engineering
West Virginia University
Vyacheslav.Akkerman@mail.wvu.edu

MS13

Formation and Structure of Quasi-Detonation Oblique Reaction Front in Annular Channel

Strong promoting effect of annular channel geometry on flame acceleration and DDT was recently found. The flame area at the bend part increases several times without any impact of turbulence. A series of experiments on premixed burning in annular channels of thickness 1-, 3-, 5-cm and outer dimeter 28 cm is performed. The test channel was filled with 15-85% H2/O2 premixtures at normal pressure and temperature, and then ignited near the outer wall. Initially spherical, a then-oblique reaction front propagates along the outer wall. Different inner and outer channel curvature provides additional flame stretching, which leads to a drastic increase in the flame surface and rapid acceleration to a near-sonic (350-650m/s) speed. For most reactive mixtures (40-80% H2), the tangential flame velocity reaches the Chapman-Jouguet (CJ) detonation velocity (2100-3400m/s). The complex formed by an oblique shock wave and a subsonic deflagration in an annular channel is analytically investigated. The ensemble has the notable property to propagate with the CJ velocity in the circumferential direction being of intrinsic subsonic nature. The structure is discussed in detail utilizing an algebraic approach yielding an insight of apparently contradictory experimental observations of a deflagration which propagates with CJ velocity. The nature of the complex is qualitatively presented, and the mathematical relations governing the states of the gas in different areas of the ensemble are derived.

Mike Kuznetsov, Jorge Yanez
Karlsruhe Institute of Technology (KIT)
kuznetsov@kit.edu, jorge.yanez@kit.edu

MS13

Diffusion Flames and Diffusion Flame-Streets in Three Dimensional Micro-Channels

Experiments of nonpremixed combustion in microchannels exhibit different burning modes. Typically, a diffusion flame is established along/near the channel axis spanning the entire mixing layer, separating the fuel/oxidizer regions. Often, however, a periodic sequence of extinction and reignition events, termed collectively as diffusion flame-streets, is observed, with a series of separate diffusion flames, each with a tribrachial edge-flame structure that is stabilized along the channel. This work focuses on understanding the mechanism responsible for these unique observations. Numerical simulations were conducted in a thermo-diffusive limit to examine the effects of confinement and heat loss on flames in 3D microchannels with low aspect ratios. An asymptotic analysis was used to reduce the problem into a 2D one, which effectively captured 3D nature of combustion processes. Two key burning regimes were identified: (i) stable continuous diffusion flames and (ii) stable diffusion flame-streets. The transition between these regimes is demarcated primarily by the Damkohler number, defined as the diffusion-to-chemical times ratio, but is also influenced by the extent of heat loss. Occasionally within the diffusion flame-street regime, the residual mixture would reignite but fail to evolve into stationary auxiliary flames. This was observed at low flowrates for subcritical Re. The behavior is periodic in time, with a frequency dependent on the removal from criticality.

Shikhar Mohan, Moshe Matalon
Univesity of Illinois at Urbana-Champaign
smmohan2@illinois.edu, matalon@illinois.edu

MS13

DDT in Channels with Tightly Spaced Obstacles

A qualitatively new mechanism of fast flame acceleration in channels with obstacles has been recently suggested [Bychkov et al., Phys. Rev. Lett. 101, 164501 (2008)]. The advantage of the mechanism is that it does not depend on the Reynolds number. Obstacles have been used for a long time in DDT experiments for making flame acceleration stronger. It was a general belief that the Shelkin mechanism controls flame acceleration both in smooth and obstructed channels, and the main role of obstacles is to make the gas flow turbulent. In contrast to this approach, Bychkov et al. have demonstrated that the tightly spaced obstacles provide a qualitatively new mechanism of fast flame acceleration, while the role of turbulence is only supplementary. The theoretical predictions were supported by extensive numerical simulations and comparison to available experimental data. It was demonstrated that flame accelerates in the most effective way for thin obstacles with relatively small spacing in between them. Here we review the latest developments in theory and simulations of flame acceleration and DDT in channels with tightly spaced obstacles. In particular, we focus on the effect of gas compression in axisymmetric geometry. Also, we study how the obstacle length, distance between the obstacles, channel width, and thermal boundary conditions at the outer walls can modify flame propagation through a comb-shaped array of parallel thin obstacles.

Damir M. Valiev
Combustion Research Facility

Sandia National Laboratories
damir.valiev@umu.se

Orlando Ugarte
Department of Aerospace Engineering, University of Maryland
College Park, MD 20742, USA
ougartea@mix.wvu.edu

V'yacheslav Akkerman
Department of Mechanical and Aerospace Engineering
West Virginia University
Vyacheslav.Akkerman@mail.wvu.edu

MS14

Modelling of a Coaxial Lox/gh2 Injection Element under High Frequency Transverse Acoustic Velocity Forcing

A specialized high frequency combustion instability experiment, designated BKH, has been conducted at the DLR Institute for Space Propulsion. The BKH experiments operate with liquid oxygen and gaseous or liquid hydrogen propellants at supercritical conditions analogous to real rocket engines. In the experiment the response of 5 coaxial elements to imposed acoustic disturbances is observed via line of sight optical access to the combustion zone. Analysis of high speed optical data shows that the flames positioned in a pressure node are both transported by the acoustic velocity and shortened during excitation of the first transverse acoustic mode. A URANS model of a BKH injection element subjected to representative acoustic forcing has been computed using a specialized release of the DLR TAU code. This release includes a finite rate chemistry combustion model and a real gas capability for modelling cryogenic propellant injection. The single injector model reproduces the transverse transport and shortening of the flame observed experimentally. The model also provides additional insight into the deformation of the flame which could not be observed experimentally. A range of excitation amplitudes were studied to compare with previously published experimental results correlating flame length with acoustic velocity amplitude. The same trend observed experimentally was successfully reproduced by the numerical model.

Scott Beinke
German Aerospace Center (DLR)
scott.beinke@dlr.de

Daniel Banuti
Stanford University
Center for Turbulence Research
dbanuti@stanford.edu

Justin Hardi
German Aerospace Center (DLR)
justin.hardi@dlr.de

Sebastian Karl
German Aerospace Center
Goettingen
sebastian.karl@dlr.de

Michael Oschwald
German Aerospace Center (DLR)
michael.oschwald@dlr.de

Bassam Dally
The University of Adelaide
Department of Mechanical Engineering
bassam.dally@adelaide.edu.au

MS14

Experimental Test Ccases for Modelling Supercritical Combustion in Rocket Engines

Due to their challenging nature, there are a limited number of high quality experiments which can be used as test cases for modelling supercritical combustion in liquid propellant rocket engines. The German Aerospace Center (DLR), Institute for Space Propulsion operates several experimental rocket combustors with optical access which are able to provide data useful for the validation of numerical modelling. Three such experiments running cryogenic oxygen-hydrogen propellants have recently been used to generate data sets for this purpose. They range in scale from low power, single injector to high power, multi-injector configurations representative of upper stage engines. Two of the experiments are also used to study thermo-acoustic coupling phenomena relevant to combustion instabilities, introducing further aspects of complexity to the experiments and the models. These test cases are currently being modelled both internally at the DLR and by external partners in the frame of modelling workshops. Through the collaboration with modellers, the experimentalists are also addressing the challenges in comparing results from different modelling approaches with experimental data. Recent lessons learned are leading to improved methodologies to bridge the divide between the two types of data and provide better validation of the models.

Justin Hardi, Scott Beinke, Dmitry Suslov, Michael Oschwald
German Aerospace Center (DLR)
justin.hardi@dlr.de, scott.beinke@dlr.de, dmitry.suslov@dlr.de, michael.oschwald@dlr.de

MS14

Robust Treatment of Thermodynamic Nonlinearities in the Simulation of Transcritical Flows

High-pressure flows are known to be challenging to simulate due to thermodynamic nonlinearities occurring in the vicinity of the pseudo-boiling line. This study investigates the origin of this issue by analyzing the behavior of thermodynamic processes at elevated pressure and low temperature. We show that under transcritical conditions, nonlinearities significantly amplify numerical errors associated with construction of fluxes when a fully conservative approach is employed. These errors generate pressure variations that can be significant close to the pseudo-boiling line in thermodynamic space. For solvers based on a conservative system of equations, these perturbations hinder numerical stability and degrade the accuracy of predictions as non-physical turbulence may appear or unstable acoustic mode triggered. To circumvent this problem, the governing system can be reformulated to a pressure-based treatment of energy. This work presents comparisons between the pressure-based and fully conservative formulations using a progressive set of canonical cases, including a cryogenic turbulent mixing layer at rocket engine conditions. Advantages and drawbacks are discussed and new ideas on how to simulate such flows are proposed.

Guilhem Lacaze, Anthony Ruiz
Sandia National Laboratories

gnlacaz@sandia.gov, amruiz@sandia.gov

Thomas Schmitt
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr

Joseph C. Oefelein
Sandia National Laboratories
Combustion Research Facility
oefelei@sandia.gov

MS14

Diffuse Interface Transcritical Flames Models: A Comparison

Diffuse interface models are extensively used in the field of subcritical combustion and allow the numerical representation of phenomena occuring in the narrow dense-to-dilute interface. This representation may be either direct thanks to models such as Van der Waals/Korteweg models or indirect in the case of multifluids approaches. Continuous description of the interface ease computation of geometrically complex situation such as droplets fragmentation or ligament breaking. Diffuse interface models retain their relevance under supercritical conditions when the smooth dense-to-dilute transition is narrowed through stretch, motivating developpment of transcritical models. We perform an a priori comparison between extended Van der Waals/Korteweg models (P. Gaillard, V. Giovangigli, and L. Matuszewski, *A Transcritical Diffuse Interface H2/LOX flame model*, Comb. Theory Mod. 20 (2016), pp. 486–520) and multifluids approaches in term of thermodynamics, flux and entropy production. Transcritical flame structures obtained through these modellings are also compared as well as numerical efficiency of these approaches.

Vincent Giovangigli
CMAP, Ecole Polytechnique
France
vincent.giovangigli@polytechnique.fr

Lionel Matuszewski, Pierre Gaillard
ONERA
lionel.matuszewski@onera.fr, pierre.gaillard@onera.fr