IP1

Low Mach Number Simulation of Turbulent Combustion

Turbulent flames in most combustion systems occur in a low Mach number regime. By exploiting the separation of scales inherent in low Mach number flows one can potentially obtain significant computational savings, enabling a wider range of problems to be modeled. However, accurate numerical solution of the low Mach number reacting flow equations introduces a number of challenges. Here, we discuss some of these issues, focusing on treating the low Mach number constraint and the coupling of processes with different temporal scales. Results illustrating the methodology on turbulent combustion with detailed chemistry and transport will be presented.

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

IP2

Multi-scale Analysis Tools in Reacting Flows

The rapid growth of the size and complexity of kinetic mechanisms that are currently of interest demands the availability of reliable and efficient model reduction algorithms. Today, there is a large number of such algorithms available. In this talk, the fundamental concepts underlying model reduction strategies that are based on the multi-scale character of reacting flow processes will be discussed. The character of traditional methodologies (QSSA and PEA), and of more recent ones that are based on singular perturbation theory, will be analyzed on the basis of various chemical kinetic configurations.

Dimitris Goussis
National Technical University of Athens, Greece
dagoussi@mail.ntua.gr

IP3

Numerical Modeling of Pollutant Emissions with Detailed Kinetics: from Ideal Reactors to Flames

This works aims to present the activity of the research group in modeling reacting systems with hundreds of species and thousands of reactions as those typical of combustion and of pollutant emission formation, in particular. Aliphatic species up to 16 carbon atoms, aromatics up to 4 rings are all included in a mechanism of about 500 species and 15000 reactions able to simultaneously predict the formation of the main pollutants. The use of such a large mechanism requires efficient and robust numerical tools for the simulation. Some homemade codes for modeling ideal reactors, laminar flames and for postprocessing CDF computations have shown effective in developing, validating and applying large kinetic mechanisms.

Tiziano Faravelli, Alberto Cuoci, Alessio Frassoldati, Eliseo Ranzi
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
tiziano.faravelli@polimi.it, alberto.cuoci@polimi.it, alessio.frassoldati@polimi.it, eliseo.ranzi@polimi.it

CP1

Revisiting the Shrinking-Core Model of Sub-Micron Aluminum Combustion

The shrinking-core model is characterized by an interior reaction front to which O atoms and/or Al atoms diffuse through the alumina shell. Mass conservation at the front implies the generation of a displacement of the local alumina, a phenomenon that is normally ignored. We show that this displacement must necessarily lead to cracking, and it is possible that this can lead to a fractal reaction front, strongly affecting the burn time vs diameter relationship.

John D. Buckmaster
Buckmaster Research
limey@uiuc.edu

Thomas Jackson
Unversity of Ilinois at Urbana-Champaign
tlj@illinois.edu

CP1

Simulation of Refinery Gas Composition Effect on Physicochemical Properties of Combustion Products

This work analyses the effect of fuel gas composition change over physicochemical properties such as high calorific value (HCV), flame adiabatic temperature, chimney temperature and oxygen excess, using computational simulation. Four refinery gas and one natural gas streams with HCV between 800 to 2500 Btu/cubic feet were simulated; finding a significant increase in adiabatic and chimney temperature with impacts on furnace stability, energy efficiency and increase the utilization of oxygen for combustion

Lourdes I. Merino, Oscar Cala
Universidad Industrial de Santander
loumerino2@gmail.com, oscarcala20@hotmail.com

Jaqueline Saavedra
Instituto Colombiano del Petroleo
Ecopetrol
jaqueline.saavedra@ecopetrol.com.co

Viatcheslav Kafarov
Universidad Industrial de Santander
vkafarov@gmail.com

CP1

Kinetic Modeling Study of the Oxidation of Larger Methylated Hydrocarbons

Fischer-Tropsch and hydroprocessed esters and fatty acids fuels contain significant amounts of lightly branched large alkanes - which have been subject to little research. To better understand the combustion process of these fuels a kinetic mechanism for the oxidation of 2-methylheptane and larger hydrocarbons is presented. The mechanism has been generated using the software RMG and is validated against experimental data. The investigation of the effect of different basis mechanisms has been of particular interest.

Marileen L. Fischer, Elke Goos
Institute of Combustion Technology
German Aerospace Center (DLR)
marileen.fischer@dlr.de, elke.goos@dlr.de

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

CP1

Extinction Strain Rate Simulations for Three Butanol Isomers

The extinction strain rates of three butanol isomers, (n-butanol, sec-butanol and iso-butanol) were studied experimentally in a counterflow burner, and computationally using a one-dimensional numerical model. The experimental results provided an insight in how the difference between molecular structures affects combustion of the isomers in terms of their extinction through strain. Computational comparisons were also performed in the context of constant-volume ignition.

Constandinos M. Mitsingas, Dimitrios Kyritsis
University of Illinois at Urbana-Champaign
cmitsin2@illinois.edu, kyritsis@illinois.edu

CP2

Direct Numerical Simulations of Hcci and Saci with Ethanol

We conduct a 2D and 3D DNS study of an autoignitive premixture of air and ethanol. A feature of these simulations is the use of mass source and sink terms to emulate piston motion. Combustion phasing is adjusted such that peak heat release occurs after top dead center during the expansion stroke, as in a real engine. Temperature stratification is found to be the most important parameter affecting heat release, pressure rise rate and peak temperature.

Ankit Bhagatwala
Sandia National Laboratories
abhagat@sandia.gov

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

CP2

Modeling of Rcci Combustion

Since the operation of new technologies like Premixed Charge Compression Ignition decouples injection and heat-release events, no direct control over ignition is possible that is a common problem for many concepts. Dual fuel Reactivity Controlled Compression Ignition (RCCI) combustion concept is introduced to have better control over combustion-phasing. The purpose of this study is to predict counter-intuitive ignition characteristics of RCCI combustion, which is found in experiments, by using a multi-zone model with detailed chemistry.

Ulas Eguz, Bart Somers
Eindhoven University of Technology
u.eguz@tue.nl, l.m.t.somers@tue.nl

Philip de Goey
Technische Universiteit Eindhoven
l.p.h.d.goey@tue.nl

CP2

Hydrogen-Air Mixing Layer Ignition at Temperatures below Crossover

Ignition in hydrogen-air mixing layers is addressed for initial conditions of temperature and pressure that place the system below the crossover temperature associated with the second explosion limit of hydrogen-oxygen explosions. It is seen that a reduced chemical-kinetic mechanism containing only the two global steps $2H_2 + O_2 \rightarrow 2H_2O$ and $2H_2O \rightarrow H_2O_2 + H_2$, derived previously from a detailed mechanism by assuming all radicals to follow a steady-state approximation, suffices to describe accurately the ignition process. The strong temperature sensitivity of the corresponding overall rates enables activation-energy asymptotics to be used in describing the resulting thermal runaway. When the initial temperatures of both reactants differ by a relative amount that is of the order of or smaller than the inverse to the dimensionless value of the controlling activation energy, the chemical reaction occurs distributed all across the mixing layer, with the ignition time determined as a thermal-runaway in a parabolic problem. However, when the air side is sufficiently hotter, as ofter occurs in applications, ignition occurs in a thin layer close to the air-side boundary, enabling a simplified description in which the ignition time is determined by analyzing the existence of solutions to a two-point boundary-value problem involving diffusion-reaction ordinary differential equations for the temperature increase and the H_2O_2 concentration.

Eduardo Fernandez-Tarrazo
Universidad Carlos III de MAdrid
eafernan@ing.uc3m.es

Antonio Sánchez
Area de Mecánica de Fluidos
Universidad Carlos III de Madrid
asanchez@ing.uc3m.es

Amable Liñán
Escuela de Ingenieros Aeronauticos
Universidad Politécnica de Madrid
amable.linan@upm.es

Forman Williams
University of California
at San Diego
faw@ucsd.edu

CP2

Numerical Investigations of Combustion Regimes for Dual-Fuel Engines Applications

Dual-fuel concepts represent one of today's most promising way to reduce fuel consumption of internal combustion engines. There is a strong need for better understanding of the combustion process in these conditions. One proposes a numerical investigation of the reactive zone structure through various combined numerical approaches, including direct numerical simulation (DNS) of auto-ignition / premixed combustion situations and 3D simulations of dual-fuel engines with reduced combustion models for mixing and chemistry validated against DNS.

Stephane Jay
IFP Energies Nouvelles
Stephane.Jay@ifpen.fr

Haïfa Belaïd-Saleh, Cécile Pera
IFPEN
haifa.belaid@ifpen.fr, cecile.pera@ifpen.fr

CP2

Ready - a Reactive Dynamic Simulation for Hydrogen Combustion

The program READY uses molecular dynamics to simulate the mechanism of hydrogen combustion in a bulk mixture. Based on 17 accurate potential energy surfaces (PES) for systems involving oxygen and hydrogen atoms, this program simultaneously integrates all the equations of motion. Therefore one can study the time evolution of the reactive mixture under different initial conditions and follow the rate of formation and consumption of the different molecular species involved in the combustion process.

César Mogo
CIQA - Universidade do Algarve
Portugal
cfmogo@ualg.pt

João Brandão
CIQA- Universidade do Algarve
Portugal
jbrandao@ualg.pt

CP2

Acoustic Timescale Characterization of Diffusion-Free Unreacted Pocket Ignition

Volumes of unreacted fluid surrounded by combustion products are studied using numerical methods. The presented work focuses on the limit in which diffusional transport processes are negligible and heat is transported through gasdynamic heating. The acoustic timescale associated with the size of an unreacted pocket is used to distinguish between pockets that react at nearly constant pressure and constant volume conditions as well as conditions between these two limiting extrema.

Jonathan D. Regele
University of Colorado at Boulder
jregele@iastate.edu

CP3

Local Rectangular Refinement in Three Dimensions (LRR3D) with Application to Unsteady Combustion Problems

The local rectangular refinement (LRR) solution-adaptive gridding method automatically generates robust unstructured grids, uses multiple-scale discretizations, and solves coupled systems of PDES via Newton's method. LRR, which has successfully modeled numerous laminar flames in the past fifteen years, has recently been extended to unsteady applications in three spatial dimensions (LRR3D). Results will be presented for two such applications: a reaction-convection-diffusion problem having a known solution, and problems involving solid-solid alloying reactions.

Beth Anne V. Bennett, Mitchell Smooke
Yale University
Dept of Mechanical Engineering
beth.bennett@yale.edu, mitchell.smooke@yale.edu

CP3

High-Order Ceno Finite-Volume Scheme for Large-Eddy Simulation of Turbulent Premixed Flames

A novel, high-order finite-volume scheme is described for large-eddy simulations of premixed flames on three-dimensional unstructured meshes. The scheme is applied to the spatially-filtered Navier-Stokes equations governing gaseous mixtures using a pseudo-compressibility formulation and the resulting discretized equations are solved with an implicit Newton-Krylov algorithm. The proposed algorithm is applied to several laboratory-scale flames to demonstrate the predictive capabilities of the high-order solution method.

Marc R. Charest
University of Toronto Institute for Aerospace Studies
charest@utias.utoronto.ca

Clinton P. Groth
University of Toronto Institute for Aerospace Studies
Canada
groth@utias.utoronto.ca

Pierre Gauthier
Rolls-Royce Canada Limited
pierre.gauthier@rolls-royce.com

CP3

An Adaptive Deferred Correction Coupling Strategy for Low Mach Number Flows with Detailed Chemistry and Transport

We present a new computational strategy for low Mach number reacting flows based on mult-implicit spectral deferred corrections (MISDC) in an adaptive mesh refinement (AMR) framework. Compared with an existing Strang-splitting-based implementation, the MISDC implementation dramatically increases the accuracy of the numerical integration while reducing computational work. In this talk, we examine the properties of the MISDC-based scheme using representative laminar premixed and diffusion flame configurations at full laboratory scales with substantial differential transport effects.

Marc Day
Lawrence Berleley National Laboratories
MSDay@lbl.gov

Andrew Nonaka
Lawrence Berkeley National Laboratory
ajnonaka@lbl.gov

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

CP3

An Implicit-Compact Method for the Investigation of Time-Dependent Laminar Flames

We present a numerical method that seeks to combine the advantages of high order compact finite difference schemes for the simulation of time-dependent phenomena with the robustness and adaptive capability of implicit time discretization, with a view to its application to laminar combustion with detailed kinetics. Computations of several

forced and unforced oscillating jet diffusion flames permit an initial quantitative assessment of the capabilities of the implicit-compact method versus a conventional low order method.

Richard Dobbins
Yale University
Department of Mechanical Engineering
richard.dobbins@yale.edu

Mitchell Smooke
Yale University
Dept of Mechanical Engineering
mitchell.smooke@yale.edu

CP3

Parallel Implicit Adaptive Mesh Refinement Scheme for Unsteady Laminar Reactive Flows

A highly scalable parallel, implicit, finite-volume scheme with adaptive mesh refinement is proposed for the solution of the compressible, laminar flows of thermally-perfect, reactive, gaseous mixtures on multi-block, body-fitted, hexahedral mesh. Local preconditioning is used for treating the low-Mach-number regime and a Newton-Krylov-Schwarz method is used for solving the non-linear algebraic equations resulting from the spatial and temporal discretization procedures. The potential of the scheme for problems arising in combustion dynamics and thermoacoustics is demonstrated.

Clinton P. Groth
University of Toronto Institute for Aerospace Studies
Canada
groth@utias.utoronto.ca

Scott Northrup
University of Toronto
Institute for Aerospace Studies
northrup@scinet.utoronto.ca

CP3

A Robust Multigrid Method for Turbulent, Chemically Reacting Flows

The design of a robust multigrid framework for numerical simulation of turbulent, chemically reacting flows is presented. The mean-flow equations and the turbulence and chemistry model equations are advanced in time in a loosely-coupled manner, using an unconditionally positive-convergent implicit scheme (UPC) for model equations. The basic UPC scheme is extended for finite-rate chemistry models within the multigrid framework. The proposed multigrid method is nearly free of artificial stabilization, demonstrating computational savings of up to 50%.

Mark Wasserman
Technion - Israel Institute of Technology
markw@tx.technion.ac.il

Yair Mor-Yossef
Israeli CFD Center
yairm@iscfdc.co.il

Barry Greenberg
Technion, Haifa
Aerospace Engineering
aer9801@aerodyne.technion.ac.il

CP4

Studying the Impact of Shear onto the Mixing Processes of a Turbulent Stratified Flame by Means of Large Eddy Simulation

The Darmstadt stratified burner has been designed to investigate mixing, stratification and shear processes in turbulent, lean-premixed and stratified flames. Within this study two cases featuring conditions with and without shear have been investigated. The analysis is carried out by means of a conditioned evaluation of the equivalence ratio found locally at the flame and the alignment of the mixing and reaction layer providing insight into the interaction of shear and stratification.

Amer Avdic
Department of Energy and Power Plant Technology,TU Darmstadt
Graduate School of Computational Engineering, TU Darmstadt
avdic@ekt.tu-darmstadt.de

Guido Kuenne, Anja Ketelheun
TU Darmstadt
kuenne@ekt.tu-darmstadt.de,
ketelheun@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

CP4

Effects of Turbulent Reynolds Number on Turbulent Scalar Flux Transport in Premixed Flames

The transport of turbulent scalar flux in premixed flames has been analysed using DNS in which variation of the turbulent Reynolds number is achieved through independent variation of Damköhler and Karlovitz numbers. The Reynolds-averaged transport equation for the turbulent scalar flux is analysed in detail and the effects of turbulent Reynolds number on the performance of existing models for the unclosed terms have been assessed with respect to the corresponding quantities extracted from DNS data.

Robert S. Cant
University of Cambridge
rsc10@cam.ac.uk

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

CP4

Extinction and Reignition in Turbulent Nonpremixed Jet Flames with Vitiated Coflow: a One-Dimensional-Turbulence Study

We conduct a parametric study of extinction and reignition of turbulent nonpremixed flames in vitiated environments. Our goal is to characterize these phenomena under different flow Reynolds numbers and thermochemical

states. To do so, we consider the model problem of a temporal, planar, propane jet, and simulate it with the one-dimensional-turbulence model, a stochastic model that can resolve the coupling between turbulence, molecular transport and chemistry, of key importance in extinction and reignition.

Esteban Gonzalez
Combustion Science and Engineering, Inc.
estebandgj@gmail.com

David O. Lignell
Brigham Young University
davidlignell@byu.edu

Ponnuthurai Gokulakrishnan, Michael Klassen
Combustion Science & Engineering, Inc.
gokul@csefire.com, mklassen@csefire.com

CP4

Extinction Phenomena in Highly Turbulent Premixed Counterflow Flames

Studies of counterflow flames under high strain can support the analysis and modeling of local flame quenching and re-ignition. In this context, lean premixed hydrogen-air flames stabilized against counter-flowing fully burnt stoichiometric combustion products, are investigated using Direct Numerical Simulations (DNS) and experiments. This work aims to quantify the local extinction levels, examine the morphology of the extinguishing regions and assess and parameterize the driving mechanism that leads to the appearance of non-reactive regions.

Sgouria Lyra, Hemanth Kolla, Bruno Coriton, Jonathan Frank, Janine Bennett, Jacqueline Chen
Sandia National Laboratories
snlyra@sandia.gov, hnkolla@sandia.gov, brcori@sandia.gov, jhfrank@sandia.gov, jcbenne@sandia.gov, jhchen@sandia.gov

CP4

Sub-Grid Modelling of Non-Premixed Turbulent Flames

Sub-grid combustion models are often validated at moderate Reynolds numbers despite using high Reynolds numbers assumptions. Experimentally is very difficult to achieve such high Reynolds. However, it is possible to do it using numerical experiments. In the present work, we show the influence of sub-grid modelling in a methane non-premixed jet flame in the Reynolds range of 10^2-10^6. The results suggest a weak dependence on the Reynolds number if the grid is fine.

Salvador Navarro-Martinez
Department of Mechanical Engineering
Imperial College
s.navarro@imperial.ac.uk

CP4

Influence of Gas Expansion on Premixed Flame Flashback in Turbulent Channel Flow

In the present problem related to safety of stationary power generation, the coupling of gas expansion and boundary layer structure in a turbulent channel flow is addressed. Recent modeling [Gruber et al., J. Fluid Mech., DOI:10.1017/jfm.2012.345] showed that Darrieus-Landau instability is related to flashback of premixed hydrogen-air flames in the boundary layer of a turbulent channel flow. The present parametric study is focused on the influence of thermal gas expansion on the possibility of flashback.

Damir M. Valiev
Combustion Research Facility
Sandia National Laboratories
dnvalie@sandia.gov

Andrea Gruber
SINTEF Energy Research
andrea.gruber@sintef.no

Hemanth Kolla
Sandia National Laboratories
hnkolla@sandia.gov

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

Chung K. Law
Princeton University
cklaw@princeton.edu

CP5

Nonideal Diffusion in Supercritical Flows

Progresses in the efficiency of rocket engines have been obtained with high pressure combustion. Nonideal thermodynamics, transport and chemistry are involved in the corresponding supercritical combustion models. In this work, we investigate strained mixing layers between cold reactants at supercritical pressure. Classical multicomponent transport flux models lead to unphysical reactant mixing, whereas proper nonideal multicomponent transport flux models lead to dramatically different mixing layer structures due to sharpened interfaces especially near thermodynamic chemical instabilities.

Pierre Gaillard
ONERA
pierre.gaillard@onera.fr

Vincent Giovangigli
CMAP, Ecole Polytechnique
France
vincent.giovangigli@polytechnique.fr

Lionel Matuszewski
ONERA
lionel.matuszewski@onera.fr

CP5

CFD Modeling of Radiation Effects in a Partial Oxidation Flame Including Optically Thin and Dense Regions

Gasification gains significant interest for power generation and the production of chemical feedstock. A reference flame for partial oxidation, where a CH_4/CO_2 mixture is converted with O_2, is highly influenced by radiation effects as shown in [Stelzner et al., Proceed. Combust. Inst. 34, 2012]. The considered flame consists of both optically thin and optically dense regions, which require advanced radia-

tion models. A modified differential approximation (MDA) showed reasonable agreement with temperature measurements.

Franziska Hunger
Technische Universität Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
franziska.hunger@vtc.tu-freiberg.de

Bjoern Stelzner, Dimosthenis Trimis
Technische Universitaet Bergakademie Freiberg
Institute of Thermal Engineering
bjoern.stelzner@iwtt.tu-freiberg.de,
trimis@iwtt.tu-freiberg.de

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

CP5

Preferential Diffusion in Bluff-Body Stabilized Turbulent Premixed Flames

Recent experiments of Barlow et al. in a bluff-body stabilized flames revealed that atom balances are not conserved across the flame brush. C/H atom ratio computed through the measured major species showed that its values can exceed that of the original fuel by more than 10 percent. In the present paper, reacting flows in Sandia bluff-body burner are simulated using a detailed CFD code and investigated the reasons for increase in local C/H atom ratio.

Viswanath R. Katta
Innovative Scientific Solution
vrkatta@erinet.com

William Roquemore
Air Force Research Laboratory
Wright Patterson Air Force Base
melvyn.roquemore@wpafb.af.mil

CP5

Numerical Modeling of Multiphase Multicomponent Combustion in the Titanium-Boron System

We present a one-dimensional combustion model of the Titanium-Boron system, which is thermodynamically consistent. An analytical form is used to represent the equilibrium equation of state (EOS) for the solid and liquid phases of all the substances in the mixture. A multicomponent mixture EOS is created to account for the phase transitions and reaction between the individual species. We use numerical simulations to examine the results from conservation equations and compare them to experiments.

SushilKumar P. Koundinyan
University of Illinois
skumar10@illinois.edu

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

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

D. Scott Stewart
Mechanical Science and Engineering
University of Illinois at Urbana Champaign
dss@illinois.edu

CP5

A New Methodology to Incorporate Differential Diffusion in Cfd Simulations of Reactive Flows

Numerical simulations of combustion usually employ the assumptions of equal species mass diffusivities and unity Lewis number, leading to the definition of a conserved scalar, the mixture fraction, which uniquely describes the transport of species. Many combustion models have been developed within this framework. However, in case of hydrogen combustion these assumptions are no longer valid, since hydrogen diffuses much more rapidly than other chemical components. A new methodology to account for the effects of differential diffusion in CFD simulations of reactive flows is proposed.

Georgios Maragkos
Ghent University
Georgios.Maragkos@UGent.be

Pieter Rauwoens
Ghent University - UGent
Dept. of Flow, Heat and Combustion Mechanics
pieter.rauwoens@ugent.be

Bart Merci
Department of Flow, Heat and Combustion Mechanics
Gent University, Belgium
Bart.Merci@UGent.be

CP6

Dns of Soot Formation in Three Dimensional Turbulent Non-Premixed Jet Flames

A DNS of soot formation and growth in a three-dimensional n-heptane/air turbulent non-premixed jet flame is presented. Finite rate chemistry of polycyclic aromatic hydrocarbons and a bivariate distribution of soot in volume-surface sample space are employed. The soot moments are transported via a Lagrangian scheme. Lagrangian statistics show that soot growth and soot yield are strongly affected by the intermittent turbulent mixing field as well as temperature and composition history.

Antonio Attili
King Abdullah University of Science and Technology
antonio.attili@kaust.edu.sa

Fabrizio Bisetti
Kaust University
fabrizio.bisetti@kaust.edu.sa

Michael E. Mueller
Princeton University
muellerm@princeton.edu

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

CP6

Characterization of Ignition and Stabilization

Mechanisms of a Pulsating Jet Flame

Transient ignition and flame stabilization mechanisms in a pulsating vitiated jet flame are investigated using an unsteady LES flamelet model. Diagnostics is developed to analyze and quantify the ignition process. Multiple simulations over a range of operating conditions are conducted to assess the sensitivity of the model and flame-behavior to variations in coflow temperature, jet-exit conditions, and other model parameters. Model-results and comparisons with experimental data will be presented, and different stabilization scenarios are discussed.

Yuntao Chen
University of Michigan at Ann Arbor
yuntaoc@umich.edu

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

CP6

Rans Simulation of a Confined Turbulent Jet Diffusion Flame Using Conditional Source-Term Estimation

Conditional Source-term Estimation (CSE) is derived from the Conditional Moment Closure (CMC) hypothesis but does not require transport equations for conditional species concentrations. In this study, CSE is used with Trajectory Generation Low-Dimensional Manifold (TGLDM) for chemistry reduction to predict the temperature and mixture fraction profiles of a well-documented confined turbulent non-premixed methane flame. The results are compared to experimental and previous simulation results.

Jeffrey Labahn, Cecile B. Devaud
University of Waterloo
Mechanical and Mechatronics Engineering
jwllabah@uwaterloo.ca, cdevaud@uwaterloo.ca

CP6

Conditional Moment Closure Modeling of Differential Diffusion in A Turbulent Hydrogen Jet Flame

A recent formulation of the Conditional Moment Closure (CMC) model is applied to a RANS simulation of a turbulent hydrogen jet diffusion flame to model the effects of differential diffusion. Additional terms are introduced in the existing CMC transport equations for some specific species. Modeling and implementation details will be discussed. The results are compared with experimental data for a well-documented turbulent hydrogen jet flame.

Dominic Ma, Cecile B. Devaud
University of Waterloo
Mechanical and Mechatronics Engineering
mcma@uwaterloo.ca, cdevaud@uwaterloo.ca

CP6

Direct Numerical Simulation of the Stabilization Mechanism of a Turbulent Reacting Hydrogen Jet in Supersonic Cross-Flow

Three-dimensional direct numerical simulations of reacting and inert hydrogen jet in supersonic cross-flow (JICF) have been performed. A detailed chemistry mechanism is used in the reacting simulations. The JICF configuration is of relative simplicity yet retaining many features of interest, such as three-dimensionality, flame stabilization mechanism, separation and recirculation regions, wall effects, and vortical flows. The DNS results are compared with the existing experimental data, and will provide a better understanding for the physics of supersonic combustion.

Amirreza Saghafian
Stanford University
saghafian@stanford.edu

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

CP6

Influence of Boundary Layer Trip on NonSwirling and Swirling Reacting Jets Using Large Eddy Simulation

In this work, we explore the role of geometric features on the evolution of non-reacting and reacting flow in a sudden expansion with and without a swirler. A simple trip is introduced in order to represent an igniter upstream of the expansion section. LES results are compared with stereo PIV measurements. Analysis is used to explore the mechanistic role of the trip on the jet potential core, the growth of turbulent fluctuations, the recirculation zone and the combustion characteristics.

Soufien Taamallah, Konstantina Vogiatzaki, Gaurav Kewlani, santosh Shanbhogue, Ahmed F Ghoniem
Reacting Gas Dynamics Laboratory, MIT
sofiene@mit.edu, kvogiatz@mit.edu, gkewlani@mit.edu, santosh1@mit.edu, ghoniem@mit.edu

CP7

Les/dns Modelling of Mesocombustion Chambers with Arrhenius Complex Chemistry

LES/DNS are applied in a mesocombustion centimetric chamber for thermoelectricity applications. A consistent dynamic Thickened Flame Model, which permits strong local variations of the thickening factor, is developed and coupled to complex Arrhenius chemistry and transport in order to finely capture wall heat transfer, local quenching, preferential diffusion and pollutant emissions. The proposed modelling, which aims at geometric optimization of realistic mesocombustion chambers, is compared to experimental measurements and single-step chemistry DNS.

Pierre Benard
CORIA - CNRS UMR6614
pierre.benard@coria.fr

Vincent Moureau
CORIA Laboratory
Université et INSA de Rouen
vincent.moureau@coria.fr

Yves D'Angelo, Ghislain Lartigue, Marianne Cuif-Sjöstrand
CORIA - CNRS UMR6614
yves.dangelo@coria.fr, ghislain.lartigue@coria.fr, marianne.sjostrand@coria.fr

CP7

The Impact of a Les Combustion Model on the Pre-

diction of Flame Dynamics

The impact of the combustion model on the flame dynamics prediction is theoretically analysed from 1-D laminar flames. A flame response diagram is established to compare the ability of thickened and filtered flame models to capture the resolved flame response to unsteady motions, evidencing the advantage of filtering approach compared to flame thickening for a given numerical cost. This analysis is confirmed by 2-D numerical simulations of pulsed Bunsen burner laminar premixed flames.

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

Pierre Auzillon
Laboratoire EM2C, CNRS, UPR 288
Ecole Centrale Paris
pierre.auzillon@ecp.fr

Olivier Gicquel, Denis Veynante
EM2C Laboratory
Ecole Centrale Paris
olivier.gicquel@ecp.fr, denis.veynante@ecp.fr

CP7

Large Eddy Simulation of Turbulent Non-Premixed Flames Using Conditional Source-Term Estimation

Conditional Source-term Estimation (CSE) is a CMC-type turbulent combustion model where the conditional scalar field is obtained by inverting an integral equation. This model has already been successfully applied in large eddy simulation of Sandia flame D. The present contribution extends this work to Sandia flames E and F, allowing assessment of the model's performance in predicting extinction and re-ignition.

Graham R. Hendra
University of British Columbia
grrhendra@gmail.com

Kendal Bushe
Department of Mechanical Engineering
University of British Columbia
wkb@mech.ubc.ca

M. Mahdi Salehi
University of British Columbia
salehi@mech.ubc.ca

CP7

Large Eddy Simulation of Swirl Stabilized Lean Premixed Combustion Using Structured and Unstructured Solvers

Within this work the predictive capability of a joint ATF-FGM combustion modeling strategy is investigated by applying it within two academic CFD-codes where the numerical implementations and simulations have been conducted independently from each other. The target configuration is a natural gas swirl burner where the flame is surrounded by a coflow of pure air. The results are compared with a detailed set of experimental data for the velocity, species and temperature.

Guido Kuenne, Kai Aschmoneit, Anja Ketelheun
TU Darmstadt
kuenne@ekt.tu-darmstadt.de,
aschmoneit@ekt.tu-darmstadt.de,
ketelheun@ekt.tu-darmstadt.de

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

CP7

Large Eddy Simulation of Premixed Combustion Using Conditional Source-Term Estimation for Complex Geometries

Conditional source-term estimation (CSE) has been recently developed (Salehi et al. 2012) as a closure model for the large eddy simulation of premixed flames. Conditionally averaged scalars, vital for chemical rate closure via CMC hypothesis (Bilger et al. 1993), are obtained by inverting an integral equation assuming statistical homogeneity over arbitrary ensembles of points (Bushe et al. 2001). Our work extends the applicability of CSE from simple jet flames to complex geometries by modifying the Morton-ordering approach (Aftosmis et al. 2004) to form locally invertible ensembles for parallel computing.

Girish V. Nivarti, M. Mahdi Salehi
Department of Mechanical Engineering,
University of British Columbia
g.nivarti@alumni.ubc.ca, salehima@interchange.ubc.ca

W. Kendal Bushe
University of British Columbia
wkb@mech.ubc.ca

CP7

Les of a Premixed Jet Flame at Intense Turbulence

Recently, a petascale direct numerical simulation of a temporally evolving premixed jet flame has been conducted (Hawkes et al.). This DNS database is an ideal target for the validation of LES models due to its shear driven turbulence, high Reynolds number and realistic chemistry. We present LES of this configuration using a coupled levelset/progress variable model (Knudsen et al.). The focus is the evaluation of different models for the turbulent burning velocity.

Philipp Trisjono
Institut für Technische Verbrennung
RWTH Aachen
p.trisjono@itv.rwth-aachen.de

Obulescu Chatakonda
School of Photovoltaic and Renewable Energy Engineering
The University of New South Wales
obu.iitm@gmail.com

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

Evatt R. Hawkes
School of Photovoltaic and Renewable Energy Engineering
University of New South Wales

evatt.hawkes@unsw.edu.au

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

CP8

Modeling Aspects of Evaporative Fuel Scalar in Tabulated Chemistry Approach for Diesel Spray Combustion

In tabulated chemistry approach for diesel spray combustion modeling, the coupling of spray formation and reactive chemistry is performed by feeding spray source terms for solving mixture fraction and its variances, which serves as look-up variables. The evaporative fuel scalar affects mixture properties, evaporative cooling which can influence the evaporation rate of newly introduced fuel droplets and enthalpy (and temperature) calculations. In this work, this influence has been studied for both in constant volume combustion chamber and engine cycle simulations using Flamelet Generated Manifold (FGM) in STAR-CD framework.

Sridhar Ayyapureddi
Mechanical Engineering Department,
Eindhoven University of Technology, The Netherlands
s.ayyapureddi@tue.nl

Bart Somers
Eindhoven University of Technology
l.m.t.somers@tue.nl

Philip De Goey
Mechanical Engineering Department,
Eindhoven University of Technology, The Netherlands
l.p.h.d.goey@tue.nl

CP8

Influence of Fuel Staging on the Spray Characteristics in a Staged Multipoint Burner

Due to high flow and flame dynamics, lean premixed prevaporized combustors often show violent phenomena (flashback, flame extinction, thermoacoustic instabilities). Staged multipoint injection of fuel is a good candidate to control these unwanted phenomena in GT swirled burners. Large eddy simulations of a two-stage multi-injection laboratory-scale combustor are carried out to analyze its aerodynamic flow and the influence of fuel staging on the global spray behavior. Comparisons with recent experimental data are also carried out.

Sebastien Ducruix
Laboratoire EM2C
sebastien.ducruix@ecp.fr

Benoit Cheneau
SAFRAN, SNECMA
Direction YHCC
benoit.cheneau@ecp.fr

CP8

Fuel Injection: A Direct Numerical Simulation of Primary Atomization

The primary atomization is studied in moderate injection speed (Reynolds and Weber numbers are 12240 and 88880, respectively), using an adaptive VOF method based on octree meshing. Two simulations were performed for both perturbed and unperturbed inlet conditions. Moreover, in another simulation, detached droplets were removed from the domain to enable investigation of the liquid jet itself. Results are compared to the available experimental measurements and theoretical studies and good agreements were observed.

Maziyar Jalaal
Department of Mechanical Engineering, The University of British Columbia, Vancouver, Canada.
m_jalaal@yahoo.com

Kian Mehravaran
School of Engineering, The University of British Columbia,
Kelowna, Canada.
kian.mehravaran@ubc.ca

CP8

Ignition of Fuel Sprays in Laminar Mixing Layers

Vaporization and combustion in the laminar mixing layer separating a planar hot-air stream from a monodisperse spray stream has been investigated to increase understanding on autoignition leading to stabilization of high-speed spray combustion. The problem was formulated with a two-continua formalism, and the conservation equations were written in boundary-layer form with a one-step irreversible reaction with an Arrhenius rate for chemistry description. Numerical integrations reveal that, depending on the fuel diffusivity and latent heat of vaporization, combustion is established via a precipitous temperature increase at a well-defined ignition location or through a slow-propagating lean deflagration. The thermal explosion case is analyzed through activation-energy asymptotics leading to ignition distance predictions that compare well with results of numerical integrations.

Daniel Martínez-Ruiz
Grupo de Mecánica de Fluidos,
Universidad Carlos III de Madrid, Leganés, Spain
dmruiz@ing.uc3m.es

Javier Urzay
Mechanical Engineering Department,
Stanford University, Stanford, USA
jurzay@stanford.edu

Antonio Sánchez
Area de Mecánica de Fluidos
Universidad Carlos III de Madrid
asanchez@ing.uc3m.es

Forman Williams
University of California
at San Diego
faw@ucsd.edu

CP8

Modeling and Numerical Treatment of Liquid Injection Processes at High-Pressure Supercritical Conditions

Recent findings on the effects of high-pressure supercritical fluid phenomena on the fundamental physics of liquid injection processes in propulsion and power systems will be

presented. The theory and analysis will focus on development of a detailed model framework based on the Large Eddy Simulation (LES) technique that provides maximum accuracy while minimizing effects of numerical errors. Results will be anchored to key experiments through direct comparisons between measured and modeled results.

Joseph C. Oefelein, Rainer Dahms, Guilhem Lacaze, Anthony Ruiz
Sandia National Laboratories
oefelei@sandia.gov, rndahms@sandia.gov, gnlacaz@sandia.gov, amruiz@sandia.gov

CP9

Implementation of Soot Model in Flamelet Generated Manifold (FGM) for Spray H Conditions of ECN Database

Soot modelling of turbulent diesel spray combustion involves various aspects such as modelling of auto igniting spray, the establishment of diffusion like flame and heterogeneous soot formation and oxidation processes. In the current work, a soot model based on two (soot volume fraction, particle number density) equations is implemented in Flamelet Generated Manifold (FGM), which is used for reactive flow simulations in STAR-CD framework. The experimental data of Spray-H conditions from Engine Combustion Network (ECN) database is used for model validation. A prior, the soot model is applied and validated for generating phi-T maps using the homogeneous reactor chemistry database prepared at various equivalence ratios and temperature conditions.

Sridhar Ayyapureddi
Mechanical Engineering Department,
Eindhoven University of Technology, The Netherlands
s.ayyapureddi@tue.nl

Mariano Sirignano
Dipartimento di Ingegneria Chimica, Universita‘ Federico II,
Napoli, Italy
mariano.sirignano@unina.it

Bart Somers
Eindhoven University of Technology
l.m.t.somers@tue.nl

D’Anna Andrea
Dipartimento di Ingegneria Chimica, Universita‘ Federico II,
Napoli, Italy
andrae.danna@unina.it

Philip De Goey
Mechanical Engineering Department,
Eindhoven University of Technology, The Netherlands
l.p.h.d.goey@tue.nl

CP9

Budget-Analysis and Model-Assessment of Unsteady Flamelet-Formulation

An *a priori* study is performed with the objective of investigating fundamental assumptions of the flamelet formulation. To this end, a budget-analysis of the flamelet equations was evaluated from a DNS-database of a jet-in-cross-flow. This analysis shows that advective contributions along the flame-orthogonal direction can become significant in recirculation regions, where they can act as secondary ignition and flame-stabilization mechanisms. Modeling these contributions in a LES/flamelet-based combustion model is discussed and assessed *a posteriori*.

Wai Lee Chan
University of Michigan, Ann Arbor
Department of Aerospace Engineering
chanyli@umich.edu

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

Hemanth Kolla, Jacqueline Chen
Sandia National Laboratories
hnkolla@sandia.gov, jhchen@sandia.gov

CP9

Numerical Investigation of Premixed Turbulent Flame Using Tabulated Filtered Flame (F-Tacles) Combustion Model

Lean premixed combustion is recently a theme of interest in gas turbines in an effort towards nitrogen oxides, NOx, emission reduction. The combustion system involves highly unsteady interacting physical mechanisms like flame, vorticity and acoustic fluctuations. The Large Eddy Simulation (LES) is a good candidate to investigate the unsteady reacting flow field. In the present work a lean-premixed high turbulence Bunsen Type flame is numerically investigated using the Tabulated filtered flame (F-TACLES) combustion model.

Arash Hossein Zadeh
Technical University of Darmstadt Department of Energy and P
zadeh@ekt.tu-darmstadt.de

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

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

CP9

Flamelet Modeling of High Pressure Partial Oxidation

Flamelet approaches are widely used for modeling turbulence-chemistry interaction in reactive systems. These models are mainly developed for fast chemistry. Partial oxidation exhibits fast chemical time scales in the oxy-fuel flame and slow times scale in the fuel-rich post flame region. CFD results of a new flamelet approach for partial oxidation processes covering both regions are compared with experimental data from High Pressure Partial Oxida-

tion pilot plant in Freiberg.

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

Bernd Meyer
Technische Universitaet Bergakademie Freiberg
Chair of Energy Process Engineering
bernd.meyer@iec.tu-freiberg.de

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

CP9

Flamelet Modeling of Radiation Effects in a Partial Oxidation Flame

Flamelet approaches are widely used for modeling turbulence-chemistry interaction in reactive systems. These models are developed for fast chemistry. A reference flame for partial oxidation is investigated, which exhibits significant smaller time scales than a combusting system. Further, these flames are known to be highly influenced by radiation. Thus, the applicability of the flamelet approach is investigated in this flame, in particular, with regard to radiation modeling within the flamelet model.

Franziska Hunger
Technische Universität Bergakademie Freiberg
Chair of Numerical Thermo-Fluid Dynamics
franziska.hunger@vtc.tu-freiberg.de

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

CP9

A Flamelet-Based Relaxation Model for Polycyclic Aromatic Hydrocarbons

Unlike major combustion products, Polycyclic Aromatic Hydrocarbons (PAH) are characterized by long chemical time scales. To capture the coupling between fluid dynamics and chemistry, we propose a relaxation model for sooting non-premixed diffusion flames. This model is validated in 2D co-flow diffusion flames and the results are compared to those utilizing finite-rate chemistry. Then, the model is applied to reacting turbulent mixing layers to investigate the effects of turbulent transport on the yield of PAH.

Yuan Xuan, Pauline Vervisch-Kljakic, Guillaume Blanquart
California Institute of Technology
yxuan@caltech.edu, pauline@caltech.edu, g.blanquart@caltech.edu

CP10

Triple-Flame Propagation Against a Poiseuille Flow in a Porous Channel

We present a numerical study of triple-flame propagation in a non-strained two-dimensional mixing layer against a Poiseuille flow, within a thermo-diffusive model. The aim of the study is twofold. First to test recent analytical findings derived in the asymptotic limit of infinite Zeldovich number for flame fronts thin compared with their typical radius of curvature. Second to gain insight into the influence of the flow on the flame in situations where the flame in not necessarily thin. The study has focused on the effect of two main non-dimensional parameters on flame propagation, namely the flow intensity A and the flame-front thickness . The flow is found to have a negligible effect on the structure of the flame, while modifying its speed by an amount proportional to A, in agreement with the asymptotic findings. A new qualitative behaviour is found however for sufficiently large values of A, for which the flow is shown to significantly modify the flame structure for small values of . More precisely, the concavity of the triple-flame front is found to turn towards the unburnt gas for A larger than a critical value. This behaviour, which cannot be captured by an infinitely-large β asymptotic study, is found to be intimately linked to the finite values of β, which are necessarily found in any realistic model or computational study. Furthermore, the flame propagation regimes have been examined for a wide range of variations in A and ϵ. In particular, it is found that larger values of A promote combustion by increasing the ϵ-range of existence of ignition fronts, while a decrease in the value of A towards zero or negatives values increases the ϵ-range of existence of extinction fronts. These behaviours are explained by the decrease of the flame front curvature with increasing values of A.

Faisal A. Al-Malki
Department of Mathematics
Taif University
faisal_malki1@hotmail.com

Joel Daou
School of Mathematics, University of Manchester, Manchester
joel.daou@manchster.ac.uk

CP10

Simulation of Premixed Flames Using Integral Reaction Zone Modelling

We present a simulation concept for premixed flames based on an integral description of the reaction zone. A general relation between the mass burning rate through surfaces in the reactive zone and the consumption speed is derived by integral analysis. The model is implemented in OpenFOAM using a combined phase-field/level-set formulation. We present validations of the approach. Moreover we introduce an extension of the model capable of reproducing cellular flame structures in the level-set context.

Christian Bruzzese, Andreas Class
Karlsruhe Institute of Technology
Institute for Nuclear and Energy Technologies
christian.bruzzese@kit.edu, andreas.class@kit.edu

CP10

Effects of Pressure and Fuel Stream Dilution on the Structure of Axisymmetric Coflow Methane-Air Laminar Diffusion Flames: A Computational and Experimental Study

The influences of pressure and dilution on the structure of highly diluted methane-air laminar diffusion flames were investigated. Computationally, the system of fully cou-

pled, strongly nonlinear conservation equations was solved by a damped, modified Newton's method. Experimentally, chemiluminescence measurements and thin-filament ratio pyrometry methods were adopted to characterize flame-front structure and temperature fields. Through sensitivity analyses on lift-off height, the five most influential reactions were identified and the accuracy of calculated lift-off heights was improved.

Su Cao
Mechanical Engineering and Materials Science
Yale University
andy.cao@yale.edu

Beth Anne V. Bennett
Yale University
Dept of Mechanical Engineering
beth.bennett@yale.edu

Bin Ma
Mechanical Engineering and Materials Science
Yale University
bin.ma@yale.edu

Marshall Long
Yale University
Mechanical Engineering
marshall.long@yale.edu

Mitchell Smooke
Yale University
Dept of Mechanical Engineering
mitchell.smooke@yale.edu

CP10

Numerical Modeling of Laminar, Reactive Flows with Detailed Kinetic Mechanisms

In this work a numerical code for the simulation of reactive flows in laminar conditions is presented. The code is based on the OpenFOAM® framework and it is specifically conceived to manage detailed kinetic mechanisms with hundreds of species and thousands of reactions. The reliability and the accuracy of the proposed software is demonstrated through several examples of premixed and diffusive flames, compared with experimental data and analyzed from a kinetic point of view.

Alberto Cuoci, Alessio Frassoldati, Tiziano Faravelli, Eliseo Ranzi
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
alberto.cuoci@polimi.it, alessio.frassoldati@polimi.it, tiziano.faravelli@polimi.it, eliseo.ranzi@polimi.it

CP10

Simulations of Axisymmetric Coflow Laminar Diffusion Flames

A pressure-based CFD solver for simulating laminar diffusion flames has been developed based on the open-source code OpenFOAM. The solver uses mixture-averaged transport properties including differential diffusion, a semi-empirical two-equation soot model and a detailed soot model using a method of moments with interpolative closure, and an optically thin radiation model. Computed results are compared with experiment for atmospheric-pressure and high-pressure ethylene-air flames.

Adhiraj K. Dasgupta
Department of Mechanical Engineering,
The Pennsylvania State University
adhiraj@psu.edu

Somesh P. Roy
Graduate Researcher
The Pennsylvania State University
somesh@psu.edu

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

CP11

A Conditional Moment Closure Formulation for Large Eddy Simulation of Compressible Non-Premixed Turbulent Reactive Flows

A sub-grid closure model for Large Eddy Simulation (LES) of compressible non-premixed turbulent reactive flows is proposed. This is an application of the Conditional Moment Closure (CMC) method to fully compressible flows. The set of reactive Navier-Stokes equations is partitioned in two sub-sets, one filtered and solved in the physical (LES) space, the other conditionally filtered and solved in the CMC space. These sub-sets are integrated in time by means of an operator splitting technique.

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

Pietro Paolo Ciottoli, Matteo Bernardini, Sergio Pirozzoli
Dept. Mechanical and Aerospace Engineering
Univ. Rome La Sapienza
pietro.ciottoli@gmail.com, matteo.bernardini@uniroma1.it, sergio.pirozzoli@uniroma1.it

CP11

Comparison of Inflow Generation Methods for Les of Turbulent Flames

LES has become a standard tool in turbulent combustion modeling. In comparison to RANS based methods, in LES the inflow boundary conditions are always instationary and must partially resolve the turbulent spectrum according to the available grid resolution and the chosen time step. This is usally accomplished by imposing artificial turbulent motion. Three different inflow generators ([Klein, 2003], [Kempf, 2005], [Davidson, 2007]) were implemented in OpenFOAM and their performance were analyzed for turbulent diffusion flames.

Dirk Dietzel
TU Bergakademie Freiberg
Chair of Numercial Thermo-Fluid Dynamics
dirk.dietzel@student.tu-freiberg.de

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

Federico Piscaglia, Andrea Montorfano

Politecnico di Milano
Energy Department
federico.piscaglia@polimi.it, andrea.montorfano@polimi.it

Gregor Olinek, Oliver T. Stein
Universität Stuttgart
Institute for Combustion Technology
g.olenik@itv.uni-stuttgart.de,
oliver.stein@itv.uni-stuttgart.de

Andreas Kronenburg
Stuttgart University
Institute for Combustion Technology
kronenburg@itv.uni-stuttgart.de

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

CP11

Explicitly Filtered Large Eddy Simulation for Conserved Scalar Modeling of Turbulent Combustion

The grid dependence of subfilter models for large eddy simulation (LES) has prevented isolated studies of model performance, especially in the context of turbulent combustion. Explicitly filtered LES has shown to be a promising means of obtaining grid convergence by separating errors induced by finite difference approximations from those rooted in modeling assumptions. In this study, the convergence characteristics of combustion model subfilter quantities are studied via a consistent implementation in multiple canonical turbulent mixing configurations.

Colin Heye
The University of Texas at Austin
cheye@utexas.edu

Colleen Kaul
Center for Turbulence Research, Stanford University
cmkaul@stanford.edu

Venkat Raman
University of Texas at Austin
v.raman@mail.utexas.edu

CP11

Hybrid Transported-Tabulated Strategy to Downsize Detailed Chemistry for Large Eddy Simulation

A new strategy to bridge the gap between combustion detailed chemistry and LES of burners is presented: the full set of species and elementary reaction rates of the detailed mechanism are kept, but only species featuring non-zero concentration in fresh and burnt gases are transported. Intermediate chemical species are expressed resorting to their self-similar properties observed in a series of canonical combustion problems. The method is tested with success in various laminar strained flames.

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

CP11

Les of Natural Fire Propagation in a Lab-Scale Configuration

Multi-physics coupled simulations of fire propagation are performed at the laboratory flame scale and are compared to measurements to provide a comprehensive understanding of the mechanisms underlying fire propagation. In particular, the assumptions used to estimate the rate of spread are examined in detail. To the authors' knowledge, it is a first time that a LES approach solving for the flame structure and including radiative heat transfers and pyrolysis, is applied to natural fire propagation.

Melanie C. Rochoux
CERFACS - Ecole Centrale Paris
melanie.rochoux@cerfacs.fr

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

Denis Veynante, Nasser Darabiha
EM2C Laboratory
Ecole Centrale Paris
denis.veynante@ecp.fr, nasser.darabiha@ecp.fr

CP11

Large Eddy Simulation of a Gas Turbine Model Combustor

Large-eddy simulations of a gas-turbine model combustor are performed. The combustor is operated under partially-premixed conditions, and consists of a plenum, a dual-swirl nozzle, and a combustion chamber. In this investigation, a stable operating condition is considered, and available experimental data will be used for model-comparisons. A sensitivity analysis is performed to assess effects of subgrid-scale closure formulations, grid-resolution, and combustion-model on the flame and flow-field structure. A bifurcation between two distinct flame-regimes is identified and physical mechanisms that describe this mode-switching are discussed.

Yee Chee See
University of Michigan
seeyc@umich.edu

CP12

Interface Tracking of a Chemical Reacting Carbon Particle Moving in Co_2 Atmosphere

This work is devoted to the 2D numerical study of unsteady gasification of a moving cylindrical carbon particle reacting with a hot gas consisting of CO_2 and N_2 . The main feature of our simulation consists in the tracking of the solid interface reacting with the carbon dioxide following the heterogeneous reaction with a fixed-grid IBM-based method. A 1D interface tracking, which averages the burning rate over the particle surface, is compared with a 2D

interface tracking which utilizes the local burning rate.

Frank Dierich, Petr Nikrityuk
TU Bergakademie Freiberg
frank.dierich@vtc.tu-freiberg.de,
petr.nikrityuk@vtc.tu-freiberg.de

CP12

Time-Implicit Schemes with Multiresolution Adaptive Meshing for Combustion Fronts

We develop a new family of numerical methods for the simulation of combustion fronts modeled by stiff time dependent PDEs. The present approach combines high order, implicit and suitably stable temporal integration schemes with a dynamic gridding technique, based on wavelet decomposition, yielding accurate and highly compressed data representations. The efficiency of the method is assessed through the simulation of some classical configurations of laminar flames with different degrees of modeling complexity.

Max Duarte, Richard Dobbins
Yale University
Department of Mechanical Engineering
max.duarte@yale.edu, richard.dobbins@yale.edu

Mitchell Smooke
Yale University
Dept of Mechanical Engineering
mitchell.smooke@yale.edu

CP12

Implementation of Unsteady Plug Flow Reactors in Cantera

In Cantera the reactor object is zero-dimensional, hence implementation of 1-dimensional plug fow reactors is a challenge. Often this is accomplished by simulating a plug flow reactor with a series of zero-dimensional reactors, but this method breaks down when transient behavior is to be modeled. Here we will describe how to model unsteady plug flow reactors via dynamically creating and destroying zero-dimensional reactors. Several computational examples of reactor networks will be presented to illustrate the method.

David W. Mikolaitis
University of Florida
Mechanical & Aerospace Engineering
mollusk@ufl.edu

CP12

On-the-Fly Processing and Feature Extraction of Flame and Flow Properties Obtained by Direct Numerical Simulation

Modern simulation methods for turbulent combustion produce more and more raw data. Storing and transferring it is becoming the major bottleneck of the simulation process. We present our approach to this problem: analyzing the data concurrent to the simulation. By storing only extracted features and filtered information, we substantially reduce the amount of data that is permanently stored. Ways of handling inherent challenges, such as synchronization with the simulation and limited interactivity will also be discussed.

Timo Oster, Gordon Fru Atanga, Abouelmagd Abdelsamie, Dominique Thévenin
University of Magdeburg
Laboratory of Fluid Dynamics and Technical Flows
timo.oster@ovgu.de, gordon.fru@ovgu.de,
abouelmagd.abdelsamie@ovgu.de, thevenin@ovgu.de

CP12

Ember: An Unsteady Quasi-1D Flame Solver

We present Ember, a software package capable of solving a number of combustion problems represented in quasi-1D forms: steady and unsteady strained flames (premixed and diffusion), laminar flames, positively and negatively curved flames, and certain steady 2D flames. Ember implements a novel operator splitting method (Balanced Splitting) which eliminates steady-state errors. The solvers for the split terms are parallelized. Chemical properties are evaluated using Cantera. Ember is released under the open-source MIT license.

Raymond L. Speth
MIT
speth@mit.edu

William H. Green
MIT Chemical Engineering
whgreen@mit.edu

CP12

Spurious Behavior of Shock-Capturing Methods: Problems Containing Stiff Source Terms Discontinuities

The goal of this paper is to relate numerical dissipations that are inherited in high order shock-capturing schemes with the onset of wrong propagation speed of discontinuities. The manner in which the smearing of discontinuities is contained by the numerical method and the overall amount of numerical dissipation being employed play major roles. Moreover, employing finite time steps and grid spacings that are below the standard Courant-Friedrich-Levy (CFL) limit on shock-capturing methods for compressible Euler and Navier-Stokes equations containing stiff reacting source terms and discontinuities reveals surprising counter-intuitive results. Unlike non-reacting flows, for stiff reactions with discontinuities, employing a time step and grid spacing that are below the CFL limit does not guarantee a correct solution of the chosen governing equations. Instead, depending on the numerical method, time step and grid spacing, the numerical simulation may lead to (a) the correct solution, (b) a divergent solution, (c) a wrong propagation speed of discontinuities solution or (d) other spurious solutions that are solutions of the discretized counterparts but are not solutions of the governing equations. The present investigation for three very different stiff system cases confirms some of the findings of LeVeque & Yee (1990), Griffiths et al. (1992) and Lafon & Yee (1996) for a model scalar PDE. The findings might shed some light on the reported difficulties in numerical combustion and problems with stiff nonlinear (homogeneous) source terms and discontinuities in general.

Helen Yee
NASA Ames Research Center
helen.m.yee@nasa.gov

Dmitry Kotov
Stanford University, Stanford, CA
dkotov@stanford.edu

Wei Wang
Florida International University, Miami, FL
weiwang1@flu.edu}

Chi-Wang Shu
Brown University
Div of Applied Mathematics
shu@dam.brown.edu

CP13

The Contribution of Nucleation and Condensation to Soot Morphology

Modeling of soot formation is an important area of research due to the negative environmental and health effects associated with atmospheric soot. One area of particular concern is modeling of soot particle nucleation. Recent literature suggests that nucleation is a rare event, and likely to occur with five-ringed aromatics. Simulations are performed with an updated nucleation model that incorporates these findings. The effect of varying nucleation and condensation efficiencies on soot morphology is investigated.

Nickolas A. Eaves, Murray Thomson
University of Toronto
neaves@mie.utoronto.ca, thomson@mie.utoronto.ca

Seth Dworkin
Ryerson University
seth.dworkin@ryerson.ca

CP13

A Computational Study of Turbulent Nonpremixed Sooting Flames Using a High Order Method of Moments

A detailed gas-phase kinetic mechanism involving high-order polycyclic aromatic hydrocarbons, a detailed soot model (method of moments with interpolative closure), a detailed radiation model, and a novel real-time extinction diagnostic are implemented in a high-order compressible Navier-Stokes solver for direct numerical simulations of turbulent non-premixed sooting flames. The simulations provide insight on soot, radiation, and flame interactions, effect of soot on radiative heat transfer and radiative extinction at both atmospheric and high pressure configurations.

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

Vivien Lecoustre
University of Maryland
vlecous1@umd.edu

Somesh P. Roy
Graduate Researcher
The Pennsylvania State University
somesh@psu.edu

Zhaoyu Luo
University of Connecticut
luozy@engr.uconn.edu

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

Hong G. Im
University of Michigan
Department of Mechanical Engineering
hgim@umich.edu

Tianfeng Lu
University of Connecticut
tlu@uconn.edu

Kwan-Liu Ma
Department of Computer Science
University of California at Davis
ma@cs.ucdavis.edu

Ramanan Sankaran
National Centre for Computational Sciences
Oakridge National Laboratories
sankaranr@ornl.gov

Arnaud Trouve
Department of Fire Protection Engineering
University of Maryland
atrouve@umd.edu

CP13

Effects of Turbulent Combustion Modeling Errors on Soot Evolution in Turbulent Nonpremixed Jet Flames

When validating turbulent combustion models, success is usually measured by agreement with experimental data within experimental uncertainty. However, soot evolution is a slow process and even small errors in temperature, etc. within the experimental uncertainty upstream are amplified at large distances downstream where soot evolves (and other measurements are no longer available). In this talk, an algorithm is developed for propagating these upstream errors to assess the effects on the downstream evolution of soot.

Michael E. Mueller
Princeton University
muellerm@princeton.edu

Venkat Raman
University of Texas at Austin
v.raman@mail.utexas.edu

CP13

An Assessment of Aerosol-Dynamics-Based Detailed Soot Models in Laminar Premixed Flames

A set of sooting laminar premixed ethylene flames has been modeled using three detailed gas-phase chemical mechanisms and two detailed aerosol-dynamics-based soot models: a discrete sectional model (DSM) and a method of moments with interpolative closure (MOMIC). A systematic parametric study as well as numerical cost and accuracy analysis of the soot models and the gas-phase chemical mechanisms has been performed for this set of flames.

Somesh P. Roy
Graduate Researcher
The Pennsylvania State University
somesh@psu.edu

Daniel C. Haworth
Pennsylvania State University

dch12@psu.edu

CP13

Transport Properties Effects on the Combustion of Lycopodium Particles

In this paper the new combustion modeling of dust cloud particles is investigated and some new results are achieved. The structure of premixed flames propagation in lycopodium combustible system considering the uniformly distributed volatile fuel particles in an oxidizing gas mixture is analyzed. Obtaining burning velocity and flame temperature with considering the effects of the particle radius and transport properties are the aim of this paper. For investigating treatment of flame temperature and burning velocity with variation of equivalence ratio some developed codes are used. It is considered that the particles are volatile which are containing the moisture, and it is also presumed that these fuel particles vaporized first to yield a gaseous fuel. The analytical analysis is preformed in the asymptotic limit where the value of the characteristic Zeldovoich number is large. The structure of flame consists of three matched zone which are preheat zone where the rate of the gas-phase chemical reaction is small and a reaction zone where the convection and the rate of vaporization of fuel particle are too small and it can be ignored. The next lunched combustion zone is the convection zone where diffusive terms in the conservation equations are small and negligible. At last, the variations of flame characteristics for different equivalence ratio are reported.

Milad Shokouhmand
Ms.c Graduted at School of Mechanical Engineering
Iran University of Science and Technology (IUST)
milad.shokouhmand@gmail.com

Pantea Farokhzad
Ms.c Student at Iran University of Science and Technology
IUST
panteafaroukhzad@yahoo.com

Mehdi Bidabadi
Associate Professor, School of Mechanical Engineering
Iran University of Science and Technology
bidabadi@iust.ac.ir

CP13

A Fully Coupled Approach for Predicting Pollutants Formation Through Reactor Network Analysis

A truthful estimation of pollutants formation in turbulent combustion devices requires the combination of accurate CFD simulations and detailed kinetic mechanisms. In this work this is accomplished by adopting a kinetic post-processing technique, which consists in transforming a CFD simulation into a network of chemical reactors. The reliability and the accuracy of the proposed procedure is demonstrated through several examples, from lab-scale flames to more complex systems, like furnaces and combustors for aircrafts.

Alessandro Stagni
Politecnico di Milano
alessandro.stagni@mail.polimi.it

Alberto Cuoci, Alessio Frassoldati, Tiziano Faravelli, Eliseo Ranzi
Department of Chemistry, Materials, and Chemical Engineering
Politecnico di Milano
alberto.cuoci@polimi.it, alessio.frassoldati@polimi.it, tiziano.faravelli@polimi.it, eliseo.ranzi@polimi.it

CP14

Topological Segmentation for Exploring Turbulence-Chemistry Interaction

Topological segmentation of the enstrophy field is a robust method for identifying structures to explore flame-turbulence interaction. We use a fixed fraction of the maximum enstrophy for each vortex structure to identify the extents, avoiding *ad hoc* scalings to make the structure discernible. This provides desirable attributes of statistical descriptions (coherent with wide ranges) and measures such as the λ_2 criterion that are topology aware but are not selective to intensity.

Ray W. Grout
National Renewable Energy Laboratory
ray.grout@nrel.gov

P.-T. Bremer
LLNL
bremer5@llnl.gov

Gruber Andrea
SINTEF
andrea.gruber@sintef.no

J.C. Bennett
SNL
jcbenne@sandia.gov

A. Gyulassy
University of Utah
aggyulassy@ucdavis.edu ¡aggyulassy@ucdavis.edu¿

H Kolla, J.H. Chen
SNL
hnkolla@sandia.gov, jhchen@sandial.gov

CP14

On the Fractal Properties of Low Damköhler Number Flames

Direct numerical simulations of i) low Damköhler number thermochemical hydrogen-air turbulent premixed plane-jet flames with detailed chemistry and ii) thermonuclear flames in type Ia supernovae are used to analyse the fractal structure of the flames. At low Damköhler number, both data-sets exhibit fractal dimensions approaching 8/3, which is larger than previous theroretical and experimental results relating to flames at higher Damköhler number. The results are explained by theoretical arguments from two different viewpoints.

Evatt R. Hawkes
School of Photovoltaic and Renewable Energy Engineering
University of New South Wales
evatt.hawkes@unsw.edu.au

Obulesu Chatakonda
University of New South Wales
obulesu.chatakonda@unsw.edu.au

Andrew Aspden
University of Portsmouth
andrew.aspden@port.ac.uk

Alan Kerstein
Combustion Research Facility
Sandia National Laboratories, Livermore
alan.kerstein@gmail.com

Hemanth Kolla, Jacqueline Chen
Sandia National Laboratories
hnkolla@sandia.gov, jhchen@sandia.gov

CP14

Validation of a Fractal Dynamic Sgs Combustion Model for Les by Dns of Turbulent Jet and V-Shape Premixed Flames

A dynamic subgrid scale combustion model which is based on fractal characteristics of turbulent premixed flames is proposed. The model is verified by using filtered direct numerical simulation (DNS) data of hydrogen-air turbulent premixed flames: planar, jet and V-shape flames. The predictions of the developed model agree quite well with the DNS data. The superiority of the model to other conventional models in terms of accuracy is demonstrated.

Katsuhiro Hiraoka, Itaru Yoshikawa, Naoya Fukushima, Masayasu Shimura
Tokyo Institute of Technology
khiraoka@navier.mes.titech.ac.jp,
iyoshikaw@navier.mes.titech.ac.jp,
nfukushim@navier.mes.titech.ac.jp,
mshimura@navier.mes.titech.ac.jp

Mamoru Tanahashi
Dep. of Mechanical and Aerospace Eng.
Tokyo Institute of Technology
mtanahas@mes.titech.ac.jp

Toshio Miyauchi
Dep. of Mechano-Aerospace Eng.
Tokyo Institute of Technology
tmiyauch@mes.titech.ac.jp

CP14

Scale-Space Analysis of Turbulent Flame Structures

We present and compare analyses of two fully-resolved numerical simulations of the flame interaction with steadily driven turbulence in the thin-reaction zone regime. We perform a scale-space analysis of the fuel mass fraction to characterize the turbulent flame structure as a function of length scale and time. The scaling behavior of the turbulent flame structure as well as its variability depends on the turbulent intensity. A universal scaling behavior is not observed.

Aaron P. Jackson
Self
aaron.jackson.ctr@nrl.navy.mil

Alexei Poludnenko, Elaine Oran
Naval Research Laboratory
alexei.poludnenko.up@nrl.navy.mil,
elaine.oran@nrl.navy.mil

CP14

Simulation of Premixed Flames As Gasdynamic Discontinuities in Artificial Turbulent Flow Fields

We present simulations of premixed flames modelled as gasdynamic discontinuities in artificially generated two and three-dimensional turbulent flow fields. Results are evaluated with regard to flame wrinkling effects and turbulent kinetic energy production. Moreover we discuss the influence of the perturbative correction of the Rankine Hugoniot jump conditions, an effect which is usually neglected in simulations of premixed flames within the G-equation context. Finally we comment the surface of discontinuity within the flame structure.

Sabine Strein, Christian Bruzzese, Andreas Class
Karlsruhe Institute of Technology
Institute for Nuclear and Energy Technologies
sabine.strein@kit.edu, christian.bruzzese@kit.edu,
andreas.class@kit.edu

CP15

Comparison of Reduced Chemistry and Tabulated Chemistry Modeling in Large-Eddy Simulation of a Two-Phase Experimental Burner

Large-Eddy Simulation of a two-phase kerosene-air flame in an experimental burner is investigated. Two different approaches of simplified chemistry modeling, reduced scheme and tabulated method, are considered and coupled to the same gaseous solver using the same Eulerian approach for the liquid phase. Liquid phase dynamics and droplet dispersion are first compared with experiments in both approaches. The impact of chemistry on the spray flame structure is then analysed.

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

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

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

Nasser Darabiha
EM2C Laboratory
Ecole Centrale Paris
nasser.darabiha@ecp.fr

CP15

Detailed Numerical Study of the Effects of Oh and O2 Oxidation Rates on Soot Formation in Flames

Collisions of soot particles with OH radicals and O2 molecules are the primary mechanisms through which soot is oxidized. Therefore, the oxidation rates of OH and O2 are the key parameters to accurately model the consumption of soot. However, one needs a proper understanding of which oxidation pathways contribute significantly to soot oxidation in order to develop an effective model. This study aims to numerically investigate the contribution of O2 and OH to soot oxidation.

Ali Khosousi
PhD Candidate

ali.khosousi@ryerson.ca

Murray Thomson
University of Toronto
thomson@mie.utoronto.ca

Seth Dworkin
Ryerson University
seth.dworkin@ryerson.ca

CP15

Fundamental Issues in Combustion Using Implicit Simulations with Realistic Chemistry: Flame-Pressure Interactions and Stretched Flame Speed

Fundamental issues in combustion may be invstigated in great detail with computational methods that couple the unsteady compressible flow to the comprehensive chemistry and multicomponent transport properties. An implicit method TARDIS (Transient Advection Reaction Diffusion Implicit Simulations), achieves this and important results relating to flame-pressure interactions (Malik and Lindstedt CST 182(9), 2010; CST 184(10–11), 2012), non-linear effects in stretched flame speeds (Malik CST 184(10–11), 2012) and flame structure using TARDIS will be presented.

Nadeem Malik
King Fahd University of Petroleum and Minerals
Department of Mathematics and Statistics
namalik@kfupm.edu.sa

CP15

A Tabulated Chemistry Approach to Predict Transient Ignition Phenomena in Flammable Mixtures

This work demonstrates a tabulated chemistry approach to analyze ignition phenomena in a premixed environment of engine relevant heavy fuels with air. The numerical framework and construction of the chemistry table are described followed by validation studies consisting of ignition in: a 0-D homogeneous reactor, a 1-D reactor with heat diffusion from a hot wall, and a 2-D reactor with an inert hot surface. Comparisons are presented with detailed chemistry calculations and available experimental data.

Shyam K. Menon, Philipp Boettcher
California institute of technology
smenon@caltech.edu, philipp@caltech.edu

Brian Ventura
Georgia institute of technology
brian.ace.ventura@gmail.com

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

Joseph E. Shepherd
California Inst of Technology
jeshep@galcit.caltech.edu

CP15

A Fast Method for Decoupled Species and Reaction Reduction in Adaptive Chemistry Combustion Simulations

We present a new mechanism reduction method designed for Adaptive Chemistry (i.e. dynamic spatial distribution of smaller, locally-valid reduced mechanisms over the course of a simulation, rather than a single, larger reduced mechanism). Species and reaction reductions are decoupled, enabling independent optimization of each. The method is fast and can be applied on-the-fly. It also applies intuitive and effective error controls. We present results of application in combustion CFD.

Oluwayemisi Oluwole, Graham Goldin
ANSYS, Inc.
luwi.oluwole@ansys.com, graham.goldin@ansys.com

CP15

Identification of Critical Chemical Processes for Limit Flame Phenomena

A systematic method based on bifurcation analyses was developed to identify important chemical species and reactions that control limit flame phenomena, including ignition and extinction, in steady-state flames involving complex chemical kinetics. These important reactions and species were then utilized to construct compact mechanisms that can mimic the detailed mechanisms for accurate prediction of flame ignition and extinction. Dimethyl ether (DME) was employed to demonstrate this method for computational diagnostics and reduction of complex chemistry.

Ruiqin Shan, Tianfeng Lu
Department of Mechanical Engineering
University of Connecticut
ruiqin.shan@engr.uconn.edu, tlu@engr.uconn.edu

CP16

Large-Scale Modulation of Turbulent Bunsen Flames

The effects of a spatial time-modulated forcing acting on a turbulent Bunsen flame are investigated using direct numerical simulations of the Navier-Stokes equations with parametrized chemistry. We adopt a superposition of spatially filtered small-scale random fluctuations and a structured large-scale flow to perturb the flame. The premixed Bunsen flame is agitated by this combined large- and small-scale perturbations at the inflow plane of a rectangular domain of size $L \times L \times 2L$ in the x, y and streamwise z direction. The inflow perturbation is focused on a region of size $L \times D$ in the x and y direction. A parametric variation is carried out considering different modulation frequencies for the imposed large-scale perturbation. We focus the effects of this external forcing on global characteristics of the turbulent flame, i.e., the flame surface density and the turbulent burning velocity.

Thiago Cardoso De Souza
Technische Universiteit Eindhoven
Mechanical Engineering Department - Combustion Group
t.cardoso.de.souza@tue.nl

Rob Bastiaans
Technische Universiteit Eindhoven
r.j.m.bastiaans@tue.nl

Bernard Geurts
Twente University

Multiscale Modeling and Simulation - Applied Mathematics
b.j.geurts@utwente.nl

Phillip de Goey
Technische Universiteit Eindhoven
Mechanical Engineering Department - Combustion Group
l.p.h.d.goey@tue.nl

CP16

DNS of Turbulent Oxy-fuel Flames – Effects of Differential and Thermal Diffusion

For combustion, using oxygen enriched oxidizers instead of air has several advantages, e.g. increased thermal efficiency, increased flame stability and reduced NOx emissions. Due to high flame temperatures effects of differential and thermal diffusion have to be investigated. Especially in turbulent flame regimes it is unclear how diffusion processes are affected by turbulence. In this work a detailed analysis of diffusion processes in turbulent oxy-methane flames is presented using DNS with detailed chemical kinetics.

Felix Dietzsch
TU Bergakademie Freiberg
Felix.Dietzsch@vtc.tu-freiberg.de

Gordon Fru, Dominique Thevenin
Otto-von-Guericke Universitaet
Lab. of Fluid Dynamics and Technical Flows
gordon.fru@ovgu.de, thevenin@ovgu.de

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

CP16

Application of a PDF Method and DNS to Ignition Processes in Transient Turbulent Jets

In this project a standalone Probability Density Function (PDF) method is used to study ignition of premixed hydrogen-air mixtures by hot turbulent transient jets. Since it is difficult to measure experimentally the relevant turbulence features under highly unsteady conditions, Direct Numerical Simulations (DNS) with detailed physico-chemical models are employed to validate the PDF calculations. Therefore, the DNS and the PDF method are used to investigate the impact of turbulence on ignition probability.

Asghar Ghorbani
Physikalisch-Technische Bundesanstalt (PTB)
Bundesallee 100, 38116 Braunschweig, Germany
asghar.ghorbani@ptb.de

Gordon Fru
Univ. of Magdeburg Otto von Guericke
atanga@ovgu.de

Detlef Markus
Physikalisch-Technische Bundesanstalt (PTB)
detlef.markus@ptb.de

Dominique Thévenin
University of Magdeburg
Laboratory of Fluid Dynamics and Technical Flows
thevenin@ovgu.de

Ulrich Maas
Karlsruhe Institute of Technology
ulrich.maas@kit.edu

CP16

Investigation of Flame Kernel Expansion in a Stratified Mixture Using Dns

DNS is used to study the expansion of an air/propane flame kernel in a stratified mixture for internal combustion engine applications. An automatically reduced kinetic scheme is used to describe the chemical processes, with both equivalence ratio stratification and dilution by external/internal burned gases being considered. The stratification effect on the absolute flame speed and the burned gases dynamics is analyzed and results are compared to simpler approaches based on tabulated and single-step chemistry.

Catherine Gruselle
INSA ROUEN/ CORIA CNRS UMR 6614
catherine.gruselle@coria.fr

Perrine Pepiot
Cornell University
pp427@cornell.edu

Vincent Moureau
CORIA Laboratory
Université et INSA de Rouen
vincent.moureau@coria.fr

Yves D'Angelo
CORIA - CNRS UMR6614
yves.dangelo@coria.fr

Frédéric Ravet
Renault
frederic.ravet@renault.com

CP16

Dns of Turbulent Inhomogeneous-Reactant Premixed Flame with Complex Chemistry

DNS was carried out for an initially planar turbulent premixed flame propagating into inhomogeneously mixed reactants. The simulation uses a reduced methane-air reaction mechanism involving 18 species and 68 elementary steps. The effects of inhomogeneously-mixed reactants on the flame propagation are studied. Flame surface area enhancement is observed due to differential propagation. Unsteady effects of different displacement speed components as observed in previous one and two dimensional calculations are compared with the 3D DNS data.

Kian Min Lim, Stewart Cant
University of Cambridge
KML34@CAM.AC.UK, rsc10@cam.ac.uk

CP16

On the Finite Differences Used in Combustion DNS

Anecdotal evidence suggests that the stability of finite difference schemes used in DNS differs when simulating non-reacting and reacting flows. This talk will describe

attempts to analyse and quantify stability issues arising from model problems with heat release. Through a number of techniques, (generalized eigenvalues, GKS stability analysis and the Lyapunov equation) observations and recommendations are made regarding those finite difference schemes most able to reduce long term instability.

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

CP17

Analysis of Ignition in Coal Combustion Process Using a One-Dimensional Turbulence Model

Ignition process of coal particles under laminar and turbulent conditions are studied using an eulerian One-Dimesional Turbulence (ODT) model. Detailed particle models for vaporization, devolatilization and char oxidation/gasi?cation are fully coupled to the mass, momentum and energy governing equations in the gas phase. Detailed chemical kinetics are used in the gas phase, with a devolatilization model that includes detailed speciation. The results are compared to experimental data.

Babak Goshayeshi, James C. Sutherland
University of Utah
b.goshayeshi@gmail.com, James.Sutherland@utah.edu

CP17

The Impact of Biomass Fuels on the Volatile Flame Length During Cofiring

Pulverized coal flames have been optimized to minimize criteria pollutant emissions and attain maximum fuel conversion. This traditional method of producing power is facing new challenges due to rising CO2 emissions, criteria pollutant emissions regulations, and renewable portfolio standards. Advanced combustion methods utilizing biomass in air and oxyfuel combustion conditions are investigated with Computational Fluid Dynamics to determine the effects of volatile fraction, fuel composition, and particle size on the length of the volatile flame.

Melissa Holtmeyer, Benjamin Kumfer, Richard Axelbaum
Washington University in St. Louis
holtmeyerm@seas.wustl.edu, benjamin.kumfer@wustl.edu, axelbaum@wustl.edu

CP17

Shock-Induced Combustion of Coal Dust Layers

This paper presents two-dimensional, time-dependent simulations of the interaction of a shock wave with a layer of coal dust. Both gases and particles are treated using a continuum approach in conjunction with a kinetic theory-based model for the dense flow of granular coal particles. The resulting equations are solved using operator splitting and the flux-corrected transport algorithm. Selected results illustrating lifting and subsequent combustion of coal particles in the shock-induced flow are presented.

Ryan Houim
National Research Council Post-Doc
ryan.houim@gmail.com

Elaine S. Oran
Naval Research Laboratory
Washington, DC
oran@lcp.nrl.navy.mil

CP17

Cfd Modeling of Wood Sawdust Gasification in a Laboratory-Scale Fluidized Bed Reactor

An Eulerian multiphase approach is employed for modeling the gasification of sawdust in a lab-scale fluidized bed. The solid phase within the reactor consists of three continuous phases representing particles of wood, char and sand. The reactive system is investigated by considering chemical sub-models for wood pyrolysis, char gasification and homogenous gas-phase reactions aiming at studying the effect of the wall-boundary conditions, both for temperature and solids velocity, on the hydrodynamics of the reacting medium.

Christos Altantzis, Addison Stark, Ahmed F. Ghoniem
Massachusetts Institute of Technology
Department of Mechanical Engineering
caltantz@mit.edu, addison@mit.edu, ghoniem@mit.edu

CP17

Computational Model of Biomass Co-Firing and Pollutant Development in a Pulverized Coal-Fired Boiler

We present the key aspects of the mathematical model and numerical algorithm for simulation of combustion and pollutant development in a pulverized-coal fired boiler. Emphasis is put on the issues and used techniques related to biomass co-firing, such as the specific models of particle burnout and combustion chemistry. We demonstrate the results of a parametric study aimed at finding optimal boiler configuration with respect to minimizing the emission of mono-nitrogen oxides.

Pavel Strachota, Michal Benes, Tomas Oberhuber
Faculty of Nuclear Sciences and Physical Engineering
Czech Technical University in Prague
pavel.strachota@fjfi.cvut.cz, michal.benes@fjfi.cvut.cz, tomas.oberhuber@fjfi.cvut.cz

Vladimir Havlena
Honewell ACS AT Laboratory Prague
vladimir.havlena@honeywell.com

Robert Straka
Faculty of Metal Engineering and Industrial Computer Science
AGH University of Science and Technology, Krakow
straka@sendzimir.metal.agh.edu.pl

CP18

Modeling Anisotropic Sensitivity in Pentaerythritol Tetranitrate Using Strain Rate Dependent Detonation Rate Law

Initiation of detonation in high explosives has shown strong anisotropic sensitivity under mechanical impact. Preferred direction of crystal orientation on shock initiation has been experimentally observed in pentaerythritol tetranitrate (PETN), which resulted in dramatic difference in the detonation sensitivity upon shock compression in different directions. The ignition and growth model based on empirical observation on the pressure-dependent initiation of detonation has been widely used to date. The basis of

the model is the hot spot theory where inclusion of compressibility (or density) factor to ignite heterogeneous high explosives is noted. Since the model is independent of direction of compression, it is impossible to address sensitivity associated with preferred crystal orientation for establishing the go/no-go criteria. In this paper, we have proposed a new rate law that incorporates what has been well observed in all of PETN experiments and atomistic calculations. A general tensor notation is utilized to fully address three-dimensional effect of the strain rate dependence to the chemical kinetics of anisotropic high explosive detonation. This allows for a meaningful coupling of thermal and mechanical behavior in the global balance laws of any energetic materials.

Kihong Kim
Lawrence Livermore National Laboratory
Seoul National University
kim75@llnl.gov

Laurence E. Fried
Lawrence Livermore National Laboratory
fried1@llnl.gov

Jack J. Yoh
Seoul National University
jjyoh@snu.ac.kr

CP18

Estimating Measurement Uncertainty in the Ignition Delay Time of Methane and Ethylene Mixtures Behind Reflected Shock Waves

Calibration of a kinetic model against experimental measurements is sensitive to measurement uncertainty. We present an uncertainty analysis of ignition delay data for methane/oxygen and ethylene/oxygen mixtures. We then calibrate a small hydrocarbon oxidation model and determine which provide the greatest constraint on extinction in a perfectly-stirred reactor. We conclude that the measurement uncertainty is a factor of 2, which we show is often too large to constrain the model. The greatest constraint on the reactors behavior comes from measurements at low temperature and high pressure.

David Sheen
National Institute of Standards and Technology
david.sheen@nist.gov

Gaetano Esposito
University of Virginia
gaetano@virginia.edu

CP18

Numerical Study of Mixing and Combustion of Transverse Fuel Injection in Supersonic Mainstream

Scramjets have high specific impulse at high Mach number. Therefore, they are an indispensable technology for hypersonic vehicles. Due to a short duration of time for mixing and combustion, the control of combustion in supersonic airstream is a difficult task. Transverse injection results in rapids mixing, and, consequently enhances the flame stabilization. Therefore, mixing and combustion of transverse fuel injection in supersonic mainstream is numerically invesitgated in the current research.

Yashar Shoraka
AmirKabir University of Technology
Aerospace Department
yshoraka@yahoo.com

Sadegh Tabejamaat
AmirKabir University of Technology
Aerospace Departmen
sadegh@aut.ac.ir

CP18

A Phenomenological Study of Detonation Phenomena in Porous Mixtures of Aluminum and Teflon

The reaction mechanisms in mixtures of Aluminum and Teflon are investigated phenomenologically in order to gain better insight into the mechanisms of detonation in non-ideal mixtures. Our kinetic model describes a system of chemical reactions coupled with our hydrodynamic models for vacuum material interface tracking in order to estimate the scales of completion time of chemical reactions by comparing it with TOA of species observed by a Time of Flight Mass Spectrometry (TOFMS) experiment.

Sunhee Yoo
Department of Theoretical and Applied Mechanics
University of Illinois
syoo1@illinois.edu

Scott Stewart
University of Illinois at Urbana-Champaign
dss@illinois.edu

Sungjin Choi
Mechanical Science and Engineering
University of Illinois at Urbana Champaign
schoi11@illinois.edu

Mario Fajardo
USAF AFMC AFRL/RWMES
mario.fajardo.1@us.af.mil

CP19

Numerical Simulation of the Chemiluminescent Species in Lifted Tribrachial N-Heptane Laminar Flames with Heated Coflow

The structure and stabilization of lifted, tribrachial n-heptane laminar flames in a heated coflow of air are studied via two-dimensional reacting flow simulations. The reduced chemical mechanism for the oxidation of n-heptane is complemented with the latest chemiluminescence chemistry mechanisms for the excited state OH and CH radicals. The chemiluminescence signals are monitored as the coflow temperature is increased, transitioning the regime from propagation to autoignition in agreement with recent experiments.

Fabrizio Bisetti
Kaust University
fabrizio.bisetti@kaust.edu.sa

Mani Sarathy, Sukho Chung, Milan Toma, Sungwoo Park
KAUST
mani.sarathy@kaust.edu.sa, sukho.chung@kaust.edu.sa, milan.toma@kaust.edu.sa, sungwook.park@gmail.com

CP19

Numerical Studies of Methane-Air Mixture Ignition by Nanosecond Plasma Discharge

Ignition sequences of a methane-air mixture by Nanosecond Pulse Discharge are studied numerically. A physical model derived from experimental data is proposed to account for both external source of sensible energy due to the plasma discharge and variation of mixture composition resulted from the plasma pulse. 1-D and 2-D numerical simulations of flame ignition are performed using detailed-chemistry and multi-component transport properties. The influence of the electric field intensity and pulse duration is studied.

Maria Luis Castela
Ecole Centrale Paris
Laboratoire EM2C
maria.castela@ecp.fr

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

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

Christophe Laux
Ecole Central Paris - Laboratoire EM2C
CNRS
christophe.laux@ecp.fr

Nasser Darabiha
EM2C Laboratory
Ecole Centrale Paris
nasser.darabiha@ecp.fr

CP19

Calculation and Analysis of Electron Transport Properties Across Premixed Methane/air Flames

The variation of electron mobility and diffusivity across premixed methane/air flames under applied voltages is investigated via solutions to the Boltzmann kinetic equation. It is found that the electrons are non-thermal for electric field strengths commonly used in experiments on electric field effects on flames. The spatial variation of electrical conductivity across flames is also investigated for lean premixed flames using a simplified ion/electron chemistry comprising chemi-ionization, proton transfer, and dissociative ion/electron recombination reactions.

Mbark El Morsli
Kaust University
mbark.el.morsli@usherbrooke.ca

Jie Han
Kaust, Saudi Arabia
jie.han@kaust.edu.sa

Fabrizio Bisetti
Kaust University
fabrizio.bisetti@kaust.edu.sa

CP19

Numerical Study of the Relation Between Chemiluminescence and Heat Release in Laminar Flames

Chemiluminescence is considered an important potential diagnostics tool in combustion. In this work a numerical study on the relation of excited species concentration and heat release for various laminar premixed flames is presented. The study suggests that the ratio of OH* concentration and peak value of heat release is nearly constant for various equivalence ratios. Such ratio can provide a potential criterion to determine the equivalence ratio based on the measured OH* and heat release.

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

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

CP19

Unsteady Effects in Laminar Premixed Flames with Transverse Mixture Stratification

Laminar flame calculations were performed using a reduced methane-air reaction mechanism with 18 species and 68 elementary steps. The flame was subjected to an incoming stream of reactants with time varying equivalence ratio. It is observed that the flame exhibits hysteresis in its propagation speed, as shown in figure below. Further investigation shows time-varying correlations between the various components of the displacement speed, and these depend on the instantaneous equivalence ratio experienced by the flame.

Kian Min Lim
University of Cambridge
KML34@CAM.AC.UK

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

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

CP20

The Runge-Kutta-Legendre Method: Efficient Explicit Time Integration for Parabolic Partial Differential Equations

Stabilized Runge-Kutta time integration methods (also know as Super-Time-Stepping and Runge-Kutta-Chebyshev methods) are a novel explicit method for efficient integration of parabolic evolutionary partial differential equations. To date, these methods have been proven to be linear stable for the canonical diffusion equation. Unfortunately, when applied to non-constant coefficient or nonlinear diffusion problems, they often generate nonphysical oscillatory solutions. We introduce a class of time integration techniques, the Runge-Kutta-Legendre method, which allows for efficient time integration and simultaneously has a convex monotone property which yields non-oscillatory results for nonlinear and non-constant coefficient advection-diffusion problems. Examples from Detonation Shock Dynamics as well as compressible reactive

Navier-Stokes will be presented.

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

CP20

A Time-Accurate Pressure Projection Method for Reacting Flows

A new method is proposed to solve the pressure Poisson equation (PPE), with particular emphasis on transient, variable-density flows. Calculation of the right-hand-side of the PPE is fully explicit. The density, assumed to be a function of an arbitrary set of transported scalars, is determined by solving a non-linear system of equations at each point in the domain. The proposed method is demonstrated on several time-varying, variable-density test cases to examine its accuracy.

Amir Biglari, Tony Saad
The Institute for Clean and Secure Energy
Department of Chemical Engineering, University of Utah
amir.biglari@utah.edu, tony.saad@utah.edu

James C. Sutherland
University of Utah
James.Sutherland@utah.edu

CP20

On Spurious Numerics in Solving Reactive Equations

The objective of this paper is to investigate the difference in spurious behavior in solving the fully coupled reactive equations (without the fractional step method), comparing with the commonly used fractional step method using the Strang splitting of the reactive equations. Studies indicate that both procedures may cause an incorrect propagation speed of discontinuities if the reactive source terms are stiff. However, the Strang splitting, while introducing splitting error into the numerical procedure, is more stable than the fully coupled approach. In addition, the Strang splitting procedure exhibits more complex spurious behavior than solving the fully coupled reactive equations. The present study also includes two different ways of formulating the reactive equations. These are using all the species variables vs. using the total density and Ns-1 number of species variables (Ns is the total number of species). Solution behavior using a cut off safeguard if densities are outside the permissible range with the no safeguard option is included. The main reason for the present investigations is due to the fact that the Strang splitting procedure is widely used in combustion and reactive flow simulations. The simple cut off safeguard procedure is also commonly used by practitioners in computational physics and engineering simulations.

Dmitry Kotov
Stanford University, Stanford, CA
dkotov@stanford.edu

Helen Yee
NASA Ames Research Center
helen.m.yee@nasa.gov

Wei Wang
Florida International University, Miami, FL
weiwang1@flu.edu

Chi-Wang Shu
Brown University
Div of Applied Mathematics
shu@dam.brown.edu

CP20

Higher-Order Discontinuous Galerkin Method for Application to Realistic Combustion Problems

A higher-order Discontinuous Galerkin (DG) method is developed for application to combustion problems. The developed DG-scheme accurate describes multi-species transport under consideration of non-uniform thermal properties, accounts for detailed and stiff reaction chemistry, and is able to capture shock-discontinuities. After presenting the numerical method and demonstrating higher-order convergence properties, this algorithm is applied to combustion problems of increasing complexity, including multi-species mixing, deflagration, and detonation-systems. Advantages of the DG-method over conventional finite-difference/finite-volume schemes are discussed.

Yu Lv
Department of Aerospace Engineering
University of Michigan
lvyu@umich.edu

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

CP20

Accelerating Stiff Chemical Kinetics in Combustion Simulations Using GPUs

The evaluation of finite-rate chemical kinetics occupies the majority of the processing time in combustion simulations, due to the stiffness of the governing rate equations. Graphics processing units (GPUs) offer the massive parallelism and processing power of a CPU cluster at a fraction of the cost and power consumption, in a single device. A novel stiff solver will be presented that accelerates the solution of chemical kinetics on GPUs.

Kyle E. Niemeyer
Case Western Reserve University
kyle.niemeyer@case.edu

Chih-Jen Sung
University of Connecticut
cjsung@engr.uconn.edu

CP20

Solving Degenerate Quenching-Combustion Equations Via Exponentially Evolving Grids (eeg)

We are concerned with the numerical solution of premixed combustion model problems in rectangular spatial domains. The two-dimensional singular reaction-diffusion equations anticipated are associated with an ignition type nonlinearity involving a mathematical degeneracy at a corner point. An exponential splitting based adaptive method is proposed on the EEG. Rigorous numerical analysis are given to ensure the satisfactory effectiveness, efficiency, and numerical stability of the algorithm developed. Simulation

experiments are provided.

Qin Sheng, Matthew Beauregard
Department of Mathematics
Baylor University
Qin_Sheng@baylor.edu, matthew_beauregard@baylor.edu

CP21

Interaction of a Thin Detonation Wave with a Nonuniform Density Pattern

We present the exact linear Laplace-transform theory describing the propagation of a planar detonation front through a gaseous mixture with nonuniform density perturbations. The investigation considers the fast reaction limit in which the detonation thickness is much smaller than the size of the density perturbations. The analytical development gives the transient evolution of the detonation front and the associated downstream perturbations. The results are then used in a Fourier-analysis to consider 2D/3D isotropic density fields.

Cesar Huete
Universidad Carlos III Madrid
chuete@pa.uc3m.es

Antonio L. Sanchez, Forman Williams
University of California San Diego
asanchez@ing.uc3m.es, fwilliams@eng.ucsd.edu

CP21

Detailed Simulation of Weak and Strong Ignition-Transition Behind a Bifurcating Shock-Wave

The ignition of diluted hydrogen/oxygen mixtures in the weak and strong ignition regime behind a reflected shock are studied using detailed numerical simulations. To fully resolve all relevant scales, an adaptive mesh-refinement method in combination with a high-order discretization scheme and detailed reaction chemistry are used. Simulations at high-pressure conditions are conducted, and comparisons with experimental data are presented. Effects of boundary conditions on the ignition dynamics are investigated, and underlying ignition scenarios are analyzed.

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

Yong Sun
Department of Aerospace Engineering
University of Michigan
yosun@umich.edu

Ralf Deiterding
Oak Ridge National Laboratory
Computer Science and Mathematics Division
deiterdingr@ornl.gov

CP21

Lead Shock Velocity and Curvature Variation in Weakly Unstable Detonation

Variations in shock front velocity and curvature were measured throughout the cellular instability cycle for weakly unstable gaseous detonations. Data was obtained from direct numerical simulation and prior experiment. Shock velocity and curvature monotonically decreased throughout the cellular cycle. Growing cells exhibited large curvature spans over narrow velocity variations. Contrastingly, decaying cells were cylindrical. In velocity–curvature space, two regimes were apparent and consistent with ideal-detonation and decaying-blast profiles. The regime boundary was the Chapman-Jouguet velocity.

Scott I. Jackson, Mark Short
Los Alamos National Laboratory
sjackson@lanl.gov, short1@lanl.gov

CP21

The Simulation of a Hydrogen-Bubble Reaction Due to Shock Ignition

We simulate the combustion of a hydrogen bubble in air ignited by a shock wave in a three dimensional domain using the parallel Wavelet Adaptive Multiresolution Representation method. The compressible model includes detailed chemical kinetics, multi-component diffusion, Soret and Dufour effects, and state dependent transport properties. The physical and chemical phenomena lead to a large multiscale problem. The method is able to capture all scales using a relatively small number of degrees of freedom by adapting refinements to local demands of the solution. pWAMR provides a direct measure of the local error, and produces a verified solution.

Samuel Paolucci
University of Notre Dame
Aero/Mech Engineering
paolucci@nd.edu

Temistocle Grenga
University of Notre Dame
tgrenga@nd.edu

CP21

Vibrational Relaxation Effects on Detonation Dynamics

Recent time-dependent, multidimensional simulations of detonations in H_2-air using detailed chemical kinetics have shown substantial disagreements with the characteristics of detonation cells observed in experiments. We present evidence that slow vibrational relaxation behind the shock front, a process not ordinarily considered in combustion kinetics models, may significantly affect rates of chemical reaction and gas dynamic behavior. A model of vibrational relaxation is developed and used in numerical calculations to demonstrate these effects.

Brian D. Taylor
University of Illinois at Urbana-Champaign
bdtaylo1@gmail.com

David Kessler, Vadim N. Gamezo
Naval Research Laboratory
dakessle@lcp.nrl.navy.mil, gamezo@lcp.nrl.navy.mil

Elaine S. Oran
Naval Research Laboratory
Washington, DC
oran@lcp.nrl.navy.mil

CP21

A General Dead-Zone Predicted with the DSD

Theory

The detonation shock dynamics (DSD) theory applied to a Huygens Construction, predicts that a *dead-zone* would always exist mathematically when a detonation makes a turn, even with a smooth obstacle. The physical size of a *dead-zone* is derived to be $\sqrt{R^2 + R_c^2} - R$, with R the local radius of curvature of the boundary of the obstacle, R_c the inverse of the critical (failure) curvature on a $D_n - \kappa$ curve. In the case of a corner-turning where $R = 0$, the size of dead-zone is the same as R_c and this is observed in experiments. A dead-zone can be numerically obtained with a marked particle method to simulate the propagation of a detonation travelling over an arbitrary obstacle.

Jin Yao
Lawrence Livermore National Laboratory
yao2@llnl.gov

CP22

Large Eddy Simulation of a Supersonic Burner

Supersonic combustion has obtained increasing attention in the development of air breathing engines. However, predicting combustion characteristics in such conditions remains a challenge in CFD. In this context, both reduced chemistry and flamelet models based on detailed chemistry have been implemented in a compressible finite volume code. This study reports the LES results for a supersonic hydrogen-air burner with comparisons to experimental data. The ability of each model to reproduce supersonic combustion is then discussed.

Lisa Bouheraoua
PhD Student at CORIA (France)
lisa.bouheraoua@coria.fr

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

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

CP22

LES of MILD Combustion: Delft Jet-in-Hot-Coflow Flame

In this study, the modelling of MILD combustion using large-eddy simulation (LES) with presumed probability density functions (PDF) and Flamelet-Generated Manifolds (FGM) is investigated. This formulation is applied to the Delft jet-in-hot-coflow (DJHC) configuration. The radial variation of temperature and oxygen concentration in the coflow, peculiar to this configuration, are accounted for. Beta and top-hat PDFs are compared. Details on the modelling approach and comparisons of the LES solutions to experimental data will be presented.

Francisco E. Hernandez Perez
Eindhoven University of Technology
Mechanical Engineering Department
F.E.Hernandez.Perez@tue.nl

Jeroen van Oijen, Philip de Goey
Technische Universiteit Eindhoven
j.a.v.oijen@tue.nl, l.p.h.d.goey@tue.nl

CP22

Les Of A Premixed Jet Dns Using A Strained Flamelet Model

This study proposes a strained flamelet model for LES of high Karlovitz number premixed combustion. The model solves strained premixed flamelets, tabulates the results in terms of a progress variable and a hydrogen radical, and invokes a presumed PDF framework. Testing is performed using an LES of a premixed slot-jet DNS from Sandia National Labs. While an unstrained flamelet model poorly describes this case, the strained model captures the interactions of mixing and chemistry.

Edward Knudsen
Stanford University
edward.knudsen@gmx.us

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

Evatt R. Hawkes
School of Photovoltaic and Renewable Energy Engineering
University of New South Wales
evatt.hawkes@unsw.edu.au

CP22

LES Modeling of Stratified Flames Stabilized by Heat Losses

A Large Eddy Simulation method using tabulated chemistry is proposed. The approach is an extension of the Filtered tabulated Chemistry of Large Eddy Simulation (F-TACLES) method to take into account fuel stratification, heat losses and complex transport. The effects of these phenomena on the turbulent flame propagation speed are studied on two experimental setups representing stratified turbulent combustion from Cambridge University (SwB5) and Technische Universität Darmstadt (TSF-A).

Renaud Mercier, Pierre Auzillon
EM2C Laboratory
Ecole Centrale Paris
renaud.mercier@ecp.fr, pierre.auzillon@centraliens.net

Vincent Moureau
CORIA Laboratory
Université et INSA de Rouen
vincent.moureau@coria.fr

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

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

CP22

Large Eddy Simulation of Ignition in An Annular Multiple Injector Combustor

The present investigation is concerned with the validation of LES methodology for transient ignition calculations.

Simulations are also used to elucidate mechanisms which control the light-round sequence in a laboratory scale annular combustor. The simulation benefits from a unique experimental database gathered at EM2C on a fully transparent annular chamber equipped with 16 premixed swirled injectors. The F-TACLES combustion model is employed for its ability to properly represent turbulent flame propagation in an LES framework.

Thomas Schmitt, Maxime Philip, Matthieu Boileau, Ronan Vicquelin, Jean-Francois Bourgoin, Daniel Durox, Sébastien Candel
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr, maxime.philip@ecp.fr, matthieu.boileau@ecp.fr, ronan.vicquelin@ecp.fr, jean-francois.bourgouin@ecp.fr, daniel.durox@ecp.fr, sebastien.candel@ecp.fr

CP22

Assessment of Conditional Source-Term Estimation Method for Large-Eddy Simulation of Turbulent Premixed Flames

The conditional source-term estimation (CSE) is applied to the modelling of subfilter-scale turbulence-chemistry interactions in large-eddy simulation (LES) of turbulent premixed laboratory-scale Bunsen-type flames. Detailed comparisons are made between the CSE method and LES solutions obtained using a laminar flamelet type model: the presumed conditional moment with tabulated chemistry (PCM-FPI) model. The LES predictions are also compared to available experimental data for the Bunsen flames at various equivalence ratios and turbulence intensities.

Nasim Shahbazian
University of Toronto
shahbazian@utias.utoronto.ca

M. Mahdi Salehi
Department of Mechanical Engineering,
University of British Columbia
salehima@interchange.ubc.ca

Clinton P. Groth
University of Toronto Institute for Aerospace Studies
Canada
groth@utias.utoronto.ca

W. Kendal Bushe
The University of British Columbia
wkb@mail.ubc.ca

CP23

Non-Linear and Linear Stability of Pulsating Overdriven Detonation with a Chain-Branching Kinetics Model

The non-linear and linear dynamics of gaseous overdriven one-dimensional detonations with a two-step chain-branching kinetic mechanism are investigated. Stable detonations are obtained when the (state insensitive) main heat release layer is longer than the initial induction layer. Linear analyses reveal a destabilizing effect (with respect to the limiting Chapman-Jouguet case) for small overdrive. The corresponding nonlinear dynamics of the pulsating detonation are studied.

Carlos Chiquete, Mark Short
Los Alamos National Laboratory
chiquete@lanl.gov, short1@lanl.gov

CP23

Two-Dimensional Pulsating Instability of High Lewis Number Flames

We present results of fully compressible Navier-Stokes simulations of pulsating flames using single-step, first-order Arrhenius kinetics. Model parameters correspond to $Ze = 9.5$, $Le = 10$, and flame Mach numbers M_L between 4.6×10^{-3} and 2.3×10^{-2}. The results show that the pulsating instability in two dimensions creates three types of transverse waves: spontaneous waves, deflagrations, and detonations. Transverse detonations become more likely as M_L increases, propagate inside the large preheat zone of the pulsating flame, and do not spread into cold material.

Vadim N. Gamezo
Naval Research Laboratory
gamezo@lcp.nrl.navy.mil

Alexei Y. Poludnenko
Laboratories for Computational Physics and Fluid Dynamics
Naval Research Laboratory, Washington, DC
apol@lcp.nrl.navy.mil

Elaine S. Oran
Naval Research Laboratory
oran@lcp.nrl.navy.mil

Forman Williams
University of California San Diego
fwilliams@eng.ucsd.edu

CP23

Response of a Transcritical Coaxial Flame Submitted to High-Frequency Transverse Acoustic Modulations

Large-eddy simulations of a transcritical coaxial jet flame are carried out to investigate the impact of high-frequency transverse acoustic modulations on the flame dynamics. The flame is placed either in a pressure node or in a pressure anti-node. Effects of the acoustic environment on the flame dynamics are revealed using phase-averaged data from the simulations. The heat release rate integrated over the chamber volume is shown to fluctuate differently depending on the acoustic oscillation features.

Thomas Schmitt, Layal Hakim
EM2C, CNRS, Ecole Centrale Paris
thomas.schmitt@ecp.fr, layal.hakim@ecp.fr

Sebastien Ducruix
Laboratoire EM2C
sebastien.ducruix@ecp.fr

Sébastien Candel
EM2C, CNRS, Ecole Centrale Paris
sebastien.candel@ecp.fr

CP23

Analytical Methods for Solving the Problem of Thermal Explosion of Polydisperse Fuel Spray Sys-

tem in the Form of Singularly Perturbed System

In our research we apply and compare between two analytical methods: the homotopy analysis method (HAM) and the method of integral invariant manifolds (MIM), for solving the problem of thermal explosion polydisperse fuel spray. The homotopy procedure enable one to control the convergence of the solutions by the so-called the h-curve. Our results includes a comparative analysis between the HAM, MIM, numerical simulations and experimental results that relate to diesel engines data.

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

Vladimir Gol'dshtein
Ben-Gurion University of the Negev
Beer-Sheva, Israel
vladimir@bgu.ac.il

Ajadi Suraju
O.A.U, Ile Ife. Nigeria.
Department of Mathematics
soajadi@yahoo.co.uk

CP23

Mathematical Investigation of Comustion Instability Due to Thermoacoustic Interaction in A Premixed Gas Turbine

In this paper a developed model of combustion instability due to the thermoacoustic interaction of gas turbine is analytically and numerically investigated, and the effect of angle of wave incidence variation on the interaction of flame and acoustic disturbance for different values of initial condition such as temperature ratio across flame and flame response parameter are compared with the existence models.

Milad Shokouhmand
Ms.c Graduted at School of Mechanical Engineering
Iran University of Science and Technology (IUST)
milad.shokouhmand@gmail.com

Pantea Farokhzad
Ms.c Student at Iran University of Science and Technology
IUST
panteafaroukhzad@yahoo.com

CP23

Direct Numerical Simulation of the Instability of Explosively Expanding Material Interfaces

The stability of material interfaces plays an important role in the point source explosion where the spatial and temporal evolution of heterogeneous explosives products exhibits jet like structures. These structures form when the explosive is mixed with the aluminum, liquid (water) and mixed liquid + aluminum particles. The possible explanation of this phenomenon is the instability which occurs at the interface between explosive products and the surrounding air. We investigate the stability of a rapidly expanding material interface and focus on the development of the two-dimensional perturbations around the contact interface by solving a system of partial differential equations using 2nd order Godunov-type Smoothing Particle Hydrodynamics (SPH) method.

Fedir Sirotkin, Min-Cheol Gwak, Jack J. Yoh
Seoul National University
fyodor@snu.ac.kr, mc4444@snu.ac.kr, jjyoh@snu.ac.kr

CP24

A Transport Equation for Flame Turbulence Interaction in Turbulent Premixed Flames

In premixed turbulent combustion scalar dissipation $\widetilde{\epsilon}_c$ and the reaction rate are directly related to *flame turbulence interaction* [Bray, K.N.C., The interaction between turbulence and combustion, Symposium (International) on Combustion (1979), pp. 223–233][Swaminathan, N and Bray, K.N.C., Effect of dilatation on scalar dissipation in turbulent premixed flames, Combustion and Flame (2005), pp. 549–565]. A new transport equation representing the degree of misalignment between the flame gradients and the eigenvectors of the strain rate is proposed in this work. The new transport equation leads to a better understanding of the flame turbulence interaction phenomenon, thus improving models for $\widetilde{\epsilon}_c$ in premixed turbulent combustion.

Umair Ahmed
University Of Manchester
umair.ahmed-2@postgrad.manchester.ac.uk

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

Alistair Revell
University Of Manchester
alistair.revell@manchester.ac.uk

CP24

Evaluation of the Subgrid Pdf of the Progress Variable of Premixed Methane and Hydrogen Flames

In numerical prediction of combustion processes most of the time averaged equations are solved, either RANS or LES. The source term of the reaction progress is unclosed. In recovering this source term frequently a beta-function PDF is used on the basis of mean values as well as standard deviation of the reaction progress, which are evaluated by transport equations. We evaluate physically comparable DNSs but for different fuels to see if this assumption is valid.

Rob Bastiaans
Technische Universiteit Eindhoven
r.j.m.bastiaans@tue.nl

Marc Day
Lawrence Berleley National Laboratories
MSDay@lbl.gov

CP24

Comparison of Statistical Properties of Advected Diffusive Scalars and Advected Propagating Fronts, and Implications for Turbulent Premixed Flame Propagation

Dissipation is governed by a Laplacian (linear) term in passive-scalar advection-diffusion but by kinematic restoration (nonlinear) in the level-set (G-equation) representa-

tion of turbulent premixed flame propagation. These small-scale dissipation mechanisms are the origins of leading-order large-scale differences between the statistics of the diffusive scalar and G fields that influence, e.g., the turbulent burning velocity and the flame-surface fractal dimension. Initial theoretical and numerical results are presented that address this dichotomy, focusing on G-field structure-function statistics.

Alan Kerstein
Combustion Research Facility
Sandia National Laboratories, Livermore
alan.kerstein@gmail.com

Jackson Mayo
Sandia National Laboratories
jmayo@sandia.gov

CP24

Statistical Behaviours of Scalar Dissipation Rate Transport Equation Terms for Turbulent Premixed Flames in the Context of Large Eddy Simulations

The statistical behaviours of the different terms of the Favre-filtered scalar dissipation rate (SDR=N_c) in turbulent premixed flames have been analysed using both simple chemistry 3D DNS data in canonical configurations and 3D detailed chemistry DNS of slot-jet flames. It has been found that the statistical behaviours of the unclosed terms of N_c are significantly affected by the filter size and a detailed scaling analysis is performed to explain the observed filter size dependences.

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

Hemanth Kolla
Sandia National Laboratories
hnkolla@sandia.gov

Y Gao
Newcastle University
y.gao@newcastle.ac.uk

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

N Swaminathan
Engineering Department
Cambridge University
ns341@cam.ac.uk

CP24

Transported Probability Density Function Modeling for High-Efficiency Compression Ignition Engines

A transported probability density function model is used to capture the influence of turbulent fluctuations in composition and temperature on mean reaction rates. Results for high-pressure, constant-volume turbulent spray combustion under engine-relevant conditions and for real engines are compared with experiment. It is shown that accounting properly for turbulent fluctuations is especially important for the low-temperature combustion environments that are of interest for advanced compression-engines.

Vivek Raja Raj Mohan, Subhasish Bhattacharjee, Daniel Haworth
Penn State University
rajav2005@gmail.com, szb158@psu.edu, dch12@engr.psu.edu

CP24

Transported Pdf Modeling for Oxy-Fuel Combustion

A transported probability density function method coupled with a stochastic photon Monte Carlo radiation model has been used to model the process of oxy-fuel (natural gas or coal) combustion. A Lagrangian particle/Eulerian mesh algorithm has been employed in this study. Temperature and composition profiles are compared with experimental data. Sensitivities of the results to model variations are explored.

Xinyu Zhao
Penn State University
xzz105@psu.edu

Daniel C. Haworth
Penn State University
Department of Mechanical Engineering
dch12@engr.psu.edu

CP25

Modeling and Numerical Simulations for Product Species Identification in Mezo-Scale Reactions of Energetic Materials

We will present our numerical algorithms in order to track vacuum interface of the product species from the reaction of nano-scale energetics that can be characterized by non-ideal equations of state of species and their reaction rates that may support non-classical detonations. A series of numerical methods are nobly connected in order to calculate the material velocity of vacuum-material interface accurately. Our scheme has been developed mainly for modeling TOFMS experiment for the identification of product species.

Sungjin Choi, Sunhee Yoo, D. Scott Stewart, Nick G. Glumac
Mechanical Science and Engineering
University of Illinois at Urbana Champaign
schoi11@illinois.edu, syoo1@illinois.edu, dss@illinois.edu, glumac@illinois.edu

CP25

Pore Collapse in Explosive Materials and the Generation of Detonations

A commonly proposed scenario for the transition from shock to detonation in an explosive material is concerned with interior void collapse. We consider a macro-scale problem which qualitatively captures well known experimental results of Borne. And we revisit the problem of pressure driven pore collapse on the micro-scale in order to obtain a better understanding of the physical mechanisms that are involved.

John D. Buckmaster
Buckmaster Research
limey@uiuc.edu

Thomas Jackson
Unversity of Ilinois at Urbana-Champaign
tlj@illinois.edu

CP25

Development of Detonation Rate Model for Selective Energetic Materials Subject to External Impact

A pressure-based chemical rate model aimed at simulating detonation phenomena of high explosive response subject to external impact and a physical procedure for determining the free parameters of the model are proposed. The depletion rate of product mass fraction (λ) sustains important physical implications which consist of an ignition term that represents formation of the hotspots due to rapid compression and a growth term that describes propagation of detonation wave in the context of Shock to Detonation Transition (SDT), as written by

$$\frac{d\lambda}{dt} = I(1-\lambda)(\frac{\rho}{\rho_0} - 1)^a + G(1-\lambda)p^b$$

Here the sensitivity parameters a, b for density and pressure, respectively are specified theoretically by the physicochemical hypotheses while the magnitude parameters, I, G are calibrated against shock initiation tests. The suggested detonation rate models for selective high explosives are tested against available rate stick data.

Bohoon Kim, Jack J. Yoh
Seoul National University
bhkim@snu.ac.kr, jjyoh@snu.ac.kr

CP25

Modeling Detonation of Heterogeneous Explosives with Embedded Inert Particles Using Detonation Shock Dynamics

Detonation Shock Dynamics provides an efficient method for studying detonation front propagation over a series of inert spherical particles embedded in a high-explosive material. Using simulation software, we observe a mesoscale model of the detonation shock wave as it passes over an array of particles. We discuss the geometry of the perturbed shock wave relative to the Huygens construction and demonstrate the periodic and convergent behavior of the system over long time scales.

Brandon A. Lieberthal, Scott Stewart, John Bdzil
University of Illinois at Urbana-Champaign
brandon.lieberthal@gmail.com, dss@illinois.edu, jbbdzil@gmail.com

CP25

Spontaneous Deflagration-to-Detonation Transition in Thermonuclear Supernovae

We present the analysis of the spontaneous deflagration-to-detonation transition (DDT) in turbulent thermonuclear flames in Type Ia supernovae - explosions of degenerate white dwarf stars in binary stellar systems. We show results of first-principles numerical calculations that are used to develop and validate a subgrid-scale model for predicting the onset of DDT in full-star calculations. We also discuss detailed properties of laminar thermonuclear deflagrations for compositions and densities, at which DDT is expected to occur.

Alexei Poludnenko, Vadim N. Gamezo
Naval Research Laboratory
apol@lcp.nrl.navy.mil, gamezo@lcp.nrl.navy.mil

Elaine S. Oran
Naval Research Laboratory
Washington, DC
oran@lcp.nrl.navy.mil

CP26

Numerical Simulation of Turbulent Hydrogen Combustion Based on Flamelet Generated Manifolds with Open Foam

The combustion method Flamelet Generated Manifolds, created in TU Eindhoven, is a reduced method for the modelling of the chemistry in the combustion simulations. FGM has become a proper solution in order to overcome the problems related with the high computing efforts in the turbulent combustion simulations. The addition of Hydrogen in the fuel mixture is important in order to evaluate the effects on biomass and coal gasification and the reducing of thermal NOx formation.

Alessio Fancello, R.J.M. Bastiaans, L.P.H. De Goey
Eindhoven University of Technology
a.fancello@tue.nl, r.j.m.bastiaans@tue.nl, l.p.h.d.goey@tue.nl

CP26

A Priori Assessment of Empirical Manifolds for Flamelet Modelling of Turbulent Premixed Combustion

Direct numerical simulation data of rectangular slot jet turbulent premixed flames of lean methane-air mixture is used to perform an a priori assessment of empirical manifolds that could be employed in RANS or LES simulations using flamelet methods. Various combinations of the independent dimensions of the manifold found in literature are considered and the aim is to confirm the presence, or lack thereof, of one and two-dimensional manifolds that form the central hypothesis of various flamelet modelling approaches.

Hemanth Kolla
Sandia National Laboratories
hnkolla@sandia.gov

Edward Knudsen
Stanford University
edward.knudsen@gmx.us

Jacqueline Chen
Sandia National Laboratories
jhchen@sandia.gov

CP26

Spatially Filtered Flamelets Applied to Premixed Turbulent Combustion

With the increasing computational power, turbulent premixed simulations often resolve almost all fluid scales falling short of resolving the chemical scales. In this context, the present work uses a simple and elegant method of spatially filtering 1D flame solutions to generate Flamelet Generated Manifold and compares well to DNS solution of a premixed Bunsen burner. Good prediction of turbulent burning speed, at reduced computational cost over DNS

and simplicity scores over other tabulated chemistry models.

Sudipto Mukhopadhyay, Rob Bastiaans, Jeroen Oijen, Philip de Goey
Technische Universiteit Eindhoven
s.mukhopadhyay@tue.nl, r.j.m.bastiaans@tue.nl, j.a.v.oijen@tue.nl, l.p.h.d.goey@tue.nl

CP26

Predicting Sooting Tendencies with a New Flamelet-Based Model

Sooting tendencies based on maximum centerline soot volume fraction are investigated using finite rate and tabulated chemistry in a 2D axisymmetric methane-air co-flow diffusion flame. Effects of differential diffusion are negligible for small-molecular-weight species, but important for heavy hydrocarbons. New 1D flamelet equations are derived to capture multidimensional convection and diffusion effects along the flame centerline. Sooting tendencies predicted by this simplified model are in good agreement with experimental results.

Yuan Xuan, Guillaume Blanquart
California Institute of Technology
yxuan@caltech.edu, g.blanquart@caltech.edu

MS1

Reaction Pathway Analysis Using Stochastic Sampling

Abstract not available at time of publication.

Rex Skodje
University of Colorado, Boulder
rex.skodje@colorado.edu

MS1

Understanding and Simplifying Chemical Processes Using Markov Chains

We propose a new approach to the simplification of chemical kinetic systems, particularly suited to systems with large uncertainties. The method measures the probability that elimination of a chemical species will influence the microstates of the system. We use a Markov process to model the transfer of atoms from one molecule to another via elementary reactions, and show that the absorption properties of the Markov chain identify chemical species to be eliminated. Preliminary results will be shown for the combustion of methane.

Luca Tosatto, Youssef M. Marzouk
Massachusetts Institute of Technology
ltosatto@mit.edu, ymarz@mit.edu

MS1

Determination of the Uncertainty of Reaction Rate Parameters

Abstract not available at time of publication.

Tamas Turanyi
Institute of Chemistry, Hungary
turanyi@chem.elte.hu

MS1

Uncertainty Quantification Applied to Combustion Experiment Design

Abstract not available at time of publication.

Hai Wang
University of Southern California
haiw@usc.edu

MS2

PCA-Based Parameterization of Composition Space in Turbulent Combustion and Implications to Modeling

A parameterization of the composition space in combustion based on principal component analysis is used and a strategy for its implementation within a multiscale turbulent combustion modeling framework is presented. The framework couples large-eddy simulation (LES) with fine-grained one-dimensional turbulence (ODT). The 1D ODT solutions are embedded in LES and solve for the principal components; while, the LES solves for the flow. Tabulation of transport and source terms is implemented using artificial neural networks.

Tarek Echekki
North Carolina State University
techekk@eos.ncsu.edu

MS2

Tabulation of Diluted Flamelets for MILD Combustion Modelling

It is now well established that reactants preheating enhances thermal efficiency and diminishes fuel consumption. To prevent an increase in NOx production, reactants may be massively diluted by burnt products to avoid hot spots and homogenize temperature gradients: it is the principle of the MILD combustion regime. Detailed kinetics and heat losses control are of paramount importance in the establishment and stabilization of this combustion process. Here, these effects are included in an extended flamelet/progress variable (FPV) tabulation approach. An analysis of flamelet responses to dilution and heat losses is done by systematically discriminating effects associated to evolutions along the control parameters dimensions. The importance of high order tabulations for MILD combustion is assessed and the predictive capabilities of the proposed tabulations highlighted. Last, Large-Eddy Simulations of laboratory scale experiments operating in MILD combustion mode are performed with a coupling with tabulations featuring various degrees of freedom. Overall results are in very good agreement with experimental data for the most complex tabulation, while discrepancies arise for lower-order chemistry lookup tables.

Jean Lamouroux
EM2C-CNRS, Ecole Centrale Paris 92295
jean.lamouroux@em2c.ecp.fr

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

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

First Nasser Darabiha
EM2C-CNRS, Ecole Centrale Paris
nasser.darabiha@em2c.ecp.fr

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

MS2

Development of Reduced Order Models Based on Principal Components and Principal Variables

Two approaches for the development of reduced-order combustion models are presented. The first, called score approach, is based on transport equations for the principal components whereas the second, called MG-PCA, is based on the resolution of transport equations for key state-space variables. The proposed models are tested a-priori using DNS and ODT data-sets, and a posteriori, using standard canonical reactor models.

Alessandro Parente
University of Pisa
alessandro.parente@utah.edu

James C. Sutherland
University of Utah
James.Sutherland@utah.edu

Ben Isaac
University of Utah & Université Libre de Bruxelles
bisaac2@gmail.com

MS2

The Identification and Use of Empirical Manifolds in Turbulent Combustion

First, we describe recent work on the identification (using PCA and MARS) of empirical manifolds from DNS databases of syngas and ethylene flames. For the ethylene flame, with 22 species, it is found that with PCA and MARS 7 and 9 dimensions, respectively, are needed to achieve 5% accuracy. Second, we discuss the different ways in which these manifolds can be used in DNS and PDF, and the different assumptions involved.

Stephen B. Pope
Cornell University
Mechanical & Aerospace Engineering
s.b.pope@cornell.edu

Yue Yang
Cornell University
yy463@cornell.edu

MS3

Chemical Kinetic Model Development Using Bayesian Variable Selection

We present a novel approach for tractable Bayesian inference of chemical kinetic models from noisy and indirect system-level data. Formulating the problem as variable selection and making use of point-mass mixture priors, our approach allows an exhaustive comparison of all models comprised of subsets of elementary reactions. Adaptive Markov chain Monte Carlo methods are used to efficiently explore the posterior distribution. We demonstrate our methodology by building kinetic models for the combustion of hydrocarbon fuels.

Nikhil Galagali, Youssef M. Marzouk
Massachusetts Institute of Technology
nikhilg1@mit.edu, ymarz@mit.edu

MS3

Quantifying Uncertainty of Ion Chemistry in Premixed Methane-air Flames

We investigate the impact of uncertainty in reaction rate parameters on the ionic structure of premixed methane-air flames. A forward propagation of uncertainty is first performed, based on an adaptive, sparse, pseudospectral projection strategy. Local and integral observables characterizing ionic concentrations are thus efficiently represented in terms of polynomial chaos representations, which are readily exploited to assess global sensitivities on rate parameters. These sensitivities are analyzed for steady premixed flames under different equivalence ratios.

Francesco Rizzi
Department of Mechanical Engineering and Materials Science
Duke University
francesco.rizzi@duke.edu

Mbark El Morsli, Fabrizio Bisetti
Kaust University
mbark.el.morsli@usherbrooke.ca,
fabrizio.bisetti@kaust.edu.sa

Omar M. Knio
Duke University
omar.knio@duke.edu

MS3

Hierarchical Validation Uncertainty Quantification of Flare Combustion Efficiency with Large Eddy Simulations

The uncertainty in predicting combustion efficiency of industrial flares has been quantified by comparing large eddy simulations (LES) with experimental data from a Helium plume and from small-scale wind tunnel flares. The V/UQ relies on a consistency constraint that requires all experiments and all simulations to be simultaneously bounded by their individual experimental uncertainty. Bayesian inference is used to predict flare combustion efficiency with uncertainty bounds where no experimental data are available.

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

Sean Smith, Jeremy Thornock, Anchal Jatale
The University of Utah
sean.t.smith@utah.edu, jeremy.thornock@utah.edu, anchal.jatale@gmail.com

MS3

Enforcing Positivity in Intrusive PC-UQ Methods for Reactive ODEs Systems

Intrusive PC-UQ Methods based on symmetric polynomials are unable to enforce the strict positivity of the state

variables (temperature, composition) in reactive systems, which might eventually lead to spurious divergence of the intrusive model. We propose a remedy which involves finding, whenever needed, the nearest positive solution state to the original state. We will demonstrate the effectiveness of the method with reference to a two-dimensional model of isothermal, chain-branching ignition.

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

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

MS4

Cavity Collapse in Elastic-plastic Materials

This presentation is concerned with modelling the collapse of cavities in solid explosives. This is achieved via the coupling of an elastoplastic solid model based on the formulation of Godunov and Romenski to a multi-phase compressible fluid model. We present the model and compare numerical results against pure fluid and elastic models.

Elizabeth R. Johnstone, Nikos Nikiforakis
Laboratory for Scientific Computing
University of Cambridge
erj28@cam.ac.uk, nn10005@cam.ac.uk

MS4

Heterogeneous Nitromethane Ignition and Transition to Detonation

This research is concerned with the numerical simulation of shock-induced cavity collapse in non-ideal condensed-phase explosives. A new underlying mathematical formulation is presented as well as results from two- and three-material simulations including the explosive, the gaseous products and an inert phase.

Louisa Michael, Nikos Nikiforakis
Laboratory for Scientific Computing
University of Cambridge
lm355@cam.ac.uk, nn10005@cam.ac.uk

MS4

Multi-phase Detonations in Elastic-plastic Confinement

Highly non-ideal explosives exhibit strong detonation velocity dependence on charge size and confiner properties. New multi-phase models have been recently formulated to address the challenges of these condensed-phase explosives with high voidage. In this work, a multi-phase model is coupled to an elastic-plastic confiner model. The resulting coupled system is used to investigate an ammonium nitrate-based mining emulsion under various confinement conditions and the results are compared against experiment.

Stefan Schoch
University of Cambridge
ss789@cam.ac.uk

Nikos Nikiforakis
Laboratory for Scientific Computing
University of Cambridge
nn10005@cam.ac.uk

MS4

Shock-induced Cavity Collapse with Reaction

A numerical study of the flow field resulting from the interaction between a planar incident shock in a reactive solid and an embedded inert gas cavity is presented. We are motivated by the need for an improved understanding of the role of embedded cavities in the initiation of reaction in a heterogeneous explosive following the application of a shock. The system is modeled as a compressible multi-fluid flow and solved numerically using a high-resolution, Godunov-type capturing scheme. The principal goal is to identify regions in which the shock-cavity interaction triggers reaction in the solid and whether the reaction is sufficient to initiate detonation.

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

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

MS4

Some Advances on Numerical Methods for Hyperbolic Balance Laws and Applications

Abstract not available at time of publication.

Eleuterio F. Toro
Department of Civil and Environmental Engineering
University of Trento, Italy
toro@ing.unitn.it

MS5

On Flame Acceleration and Deflagration-to-Detonation Transition in Tubes

Various stages of flame acceleration in smooth and obstructed tubes, starting with a finger-like flamefront, and ending with fast Chapman-Jouguet deflagration and detonation triggering are investigated, with evolution of the flame shape, velocity, acceleration rate, and velocity profiles determined in all cases. In obstructed tubes, in particular, delayed burning between the obstacles, generate a powerful jet-flow and thereby drives extremely fast acceleration. This mechanism is conceptually laminar, with turbulence playing only a supplementary role.

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

Vitaly Bychkov
Department of Physics
Umea University
vitaliy.bychkov@physics.umu.se

Chung K. Law
Dept. Mech. & Aerospace Engr.

Princeton University
cklaw@princeton.edu

Damir M. Valiev
Combustion Research Facility
Sandia National Laboratories
dnvalie@sandia.gov

MS5

On Numerical Analysis of Hydraulic Resistance Phenomena in Obstructed Channels

Hydraulic resistance and the momentum loss lie behind the multiplicity of the combustion regimes in the porous media and narrow channels. In the current study, this idea is applied to explain a sudden initial stage of flame acceleration in obstructed channels. Specifically, the influence of hydraulic resistance on flame propagation from an open end to the closed one is studied. Numerical and experimental data are analyzed yielding a simple and transparent explanation of the phenomena.

Viatcheslav Bykov
Karlsruhe University (TH)
viatcheslav.bykov@kit.edu

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

MS5

Flame Dynamics in Long Open Channels

Dynamics of premixed flames in long but finite channels, with both ends open and mixture ignited at one end, is investigated. Thermal expansion produces a continuous flow of burned gases towards the end of the channel where ignition took place. Owing to viscous drag, the flow is retarded at the walls and accelerated at the center, producing a pressure gradient that pushes the unburned gas towards the other end, with concomitant flame-stretch under appropriate conditions.

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

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

MS5

Possibility of Kinetics Study in Tubes

As a spin-off technology from microcombustion, a microflow reactor with temperature gradient is introduced by summarizing our recent studies. From weak flame regime of ordinary hydrocarbon fuels in the tube, separated triple reaction zones which correspond to the low temperature oxidation, partial oxidation to CO, and full oxidation to CO2 can be observed. Specifically, with gasoline PRF (n-heptane+iso-octane) applied, research octane number can be predicted. Possibility of combustion kinetics study for wider fuels is discussed.

Hisahi Nakamura, Takuya Tezuka, Susumu Hasegawa, Kaoru Maruta
Institute of Fluid Science
Tohoku University
nakamura@edyn.ifs.tohoku.ac.jp,
tezuka@tech.ifs.tohoku.ac.jp,
hasegawa@edyn.ifs.tohoku.ac.jp, maruta@ifs.tohoku.ac.jp

MS6

The Role of Chemical Structure in Predictions of Coal Pyrolysis and Char Conversion

The chemical structure of coals has been used to predict the pyrolysis behavior of many coals. Recently, chemical structure has been used to correlate the swelling behavior of coals during pyrolysis as a function of heating rate, as well as char conversion reactivities. These methods based on chemical structure will be reviewed, along with correlations to estimate parameters describing chemical structure.

Tom Fletcher
Brigham Young University
tom_fletcher@byu.edu

MS6

Experimental Considerations in Providing Benchmark Data on Pulverized Coal Ignition and Char Particle Burning Rates

With the development of increasingly sophisticated computational models it has become imperative for experimentalists and modelers alike to appreciate the need for careful experimental design and boundary/initial condition specification and its role in measured and modeled quantities. This is particularly true in determining fundamental coal combustion phenomena such as ignition delay and char combustion rates. These aspects are explored in detail based on the author's recent experience in measuring and modeling these quantities.

Christopher Shaddix
Sandia National Laboratories
crshadd@sandia.gov

MS6

Managing Computational Chemistry for Gasification Modeling Through the C3M Software

The National Energy Technology Laboratory has developed the Carbonaceous Chemistry for Computational Modeling (C3M) software. C3M provides easy access to validated kinetics for modeling gasification and energy related processes by linking leading databases and software packages to formatted input files for multiphase CFD codes. User friendly features, workflow, and visualization tools allow practitioners to construct complex chemistry models with confidence in a matter of minutes rather than weeks or months, saving tremendous time and money.

Dirk Van Essendelft, Chris Guenther, Mehrdad Shahnam
National Energy Technology Laboratory (NETL)
dirk.vanessendelft@netl.doe.gov,
chris.guenther@netl.doe.gov,
mehrdad.shahnam@netl.doe.gov

Nathan Weiland
West Virginia Univeristy
nathan.weiland@contr.netl.doe.gov

Richard Turton, Kiran Chaudhari
West Virginia University

richard.turton@mail.wvu.edu,
kiran.chaudhari@netl.doe.gov

Phil Nicoletti, Tingwen Li
University Research Services
philip.nicoletti@contr.netl.doe.gov, lit@contr.netl.doe.gov

Terry Jordan, Justin Weber
National Energy Technology Laboratory (NETL)
terry.jordan@netl.doe.gov, justin.weber@netl.doe.gov

MS6

Influence of Chemical Pyrolysis Product Composition on Coal Particle Ignition

Single coal particle ignition in an entrained flow reactor is investigated numerically by fully resolving the chemically reacting boundary layer flow around the particle. Using the particle heating rate, 3 pyrolysis models (CPD, FG-DVC, FLASHCHAIN) are used to compute the pyrolysis rate and the corresponding volatile species composition. The influence of the composition and the number of considered gas phase species on the computed ignition delay is investigated and the numerical results are compared to experimental data.

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

Rahul Arora
Virtuhcon, Chair of Numerical Thermo-Fluid Dynamics
rahularora090@gmail.com

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

MS7

Adaptive High-resolution Simulation of Shock-induced Unsteady Hydrogen-air Combustion

We investigate the instationary detonation-type combustion phenomena in a hydrogen-air mixture induced by the bow shock of a supersonic spherical projectile. Experiments by Lehr (1972) have confirmed a strong dependence of combustion front oscillations on the projectile velocity. We report on recent parallel simulations using the cylindrical symmetric multi-species Navier-Stokes equations with detailed chemical kinetics. Block-based Cartesian AMR is employed with MUSCL and WENO schemes; the body is represented with an embedded boundary method.

Ralf Deiterding
Oak Ridge National Laboratory
Computer Science and Mathematics Division
deiterdingr@ornl.gov

Bok Jik Lee
University of Cambridge
bjl39@cam.ac.uk

MS7

Converging Detonation in a Radial Outflow

We consider a radial supersonic outflow of a detonable gas emanating from a source. There exists a steady-state solution in which a circular converging detonation stands at some distance from the source. We analyze the structure of this solution and calculate its stability properties. Two-dimensional simulations based on the reactive Euler equations are carried out as well in order to understand the nonlinear dynamics of such detonations. The role played by frictional losses in the detonation stability is also investigated.

Aslan R. Kasimov
Division of Mathematical & Computer Sciences and Engineering
King Abdullah University of Science and Technology
aslan.kasimov@kaust.edu.sa

Svyatoslav Korneev
KAUST
svyatoslav.korneev@kaust.edu.sa

MS7

Modeling the Detonation Structure of Gaseous Detonations: What's Missing?

The present study addresses the current shortcomings in the numerical prediction of unstable detonation wave structures. A series of benchmarking experiments for the shock reflection phenomena in reactive gases are presented, with focus on Mach reflection in gases with low isentropic index and ignition behind the Mach and reflected shocks. Discrepancies of current viscous and inviscid numerical solutions stemming from inadequate chemical models, physical diffusion processes, and resolution issues are discussed.

Matei I. Radulescu
Faculty of Engineering
University of Ottawa
matei@uottawa.ca

MS7

Initiation of Viscous Detonation

The development and propagation of gaseous, viscous detonations are examined using a temporally and spatially resolved power deposition to initiate a reaction wave. The reactive Navier-Stokes equations with Arrhenius kinetics are solved. The behavior of both one-step kinetics and a detailed kinetic model are examined and compared. Qualitative structures are similar; however, one-step kinetics cannot capture the full-dynamics of detailed kinetics. An adaptive mesh refinement technique is used, which assures the finest-scale structures are resolved.

Christopher Romick
University of Notre Dame
Aerospace and Mechanical Engineering
cromick@nd.edu

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

Joseph M. Powers
University of Notre Dame

Aero/Mech Engineering
powers@nd.edu

MS8

High Fidelity Simulations of Non-Equilibrium Plasma Flows with Complex Collisional-Radiative Kinetics

We implemented a 5th-order scheme with a point-implicit solver for chemical kinetics on a GPU cluster. Previous work focused on GPU-optimization of the kinetics solver and the coupling with fluid transport. Here, we extend the scheme to thermal non-equilibrium, solving the detailed collisional-radiative (CR) kinetics. These provide a scalable testing ground for other large chemical systems, e.g. combustion of bio-diesel fuels. We show multi-dimensional calculations of ionizing shock instabilities and results of scaling studies.

Jean-Luc Cambier
Air Force Research Laboratory
Propulsion Directorate , Aerophysics
Jean-Luc.Cambier@edwards.af.mil

MS8

Accelerated Computation of Detailed Chemical Reaction Kinetics for Complex Fuels

Simulating combustion of complex hydrocarbon fuels requires the evaluation of chemical reaction terms involving a large number of species and reaction steps. The evaluation of chemical reaction terms is computationally intensive, time consuming and limits the complexity of chemical models that can be used in combustion simulations. In this talk, we present some recent software developments to utilize GPUs for accelerating the computation of detailed chemical kinetics. The talk will also present an approach for partitioning the reaction network that allows the computation to be parallelized into multiple concurrent computations and there by add an additional level of parallelism available for better utilization of the modern multicore and many core processors.

Ramanan Sankaran
National Centre for Computational Sciences
Oakridge National Laboratories
sankaranr@ornl.gov

Ray W. Grout
National Renewable Energy Laboratory
ray.grout@nrel.gov

MS8

GPU Computing for Chemical Kinetics in Combustion CFD

The Graphics Processing Unit (GPU) has recently emerged as a powerful, cost-effective supplement to the Central Processing Unit (CPU) for dramatically accelerating scientific computations. We present different approaches for exploiting the GPU for expensive chemical kinetics computations in combustion modeling. We describe opportunities in: 1) reaction rate evaluation; 2) kinetic ODE integration; and 3) hybrid CPU/GPU algorithms including a) Adaptive Chemistry+GPU, and b) CPU-based implicit/GPU-based explicit ODE integration. We show up to two orders of magnitude speedup in combustion engine simulations.

Yu Shi
Phillips 66 Research Center
Hwy 60&123, PLB-210A, Bartlesville, OK 74003
yushi92@gmail.com

Oluwayemisi Oluwole
ANSYS, Inc.
luwi.oluwole@ansys.com

William H. Green
MIT Chemical Engineering
whgreen@mit.edu

Hsi-Wu Wong
Aerodyne Research, Inc.
hwwong@aerodyne.com

MS8

Techniques for Solving Stiff Chemical Kinetics on GPUs

The implicit CVODE ODE solver and a reduced 19-species ethene combustion mechanism right-hand-side function were ported to CUDA. Implementation details and performance results will be presented using two different GPU thread mapping strategies. Performance and accuracy comparisons will be made to the baseline (CPU) CVODE solver as well as a new CUDA-based 4th-order adaptive Runge-Kutta method.

Christopher Stone
Computational Science and Engineering (LLC)
1830 N Winchester Ave., # 305, Chicago IL 60622
chris.stone@computational-science.com

MS9

Uncertainty and Sensitivity Analysis for Turbulent Combustion of Hydrogen-rich Fuels

Simulation of turbulent combustion requires physical models for turbulence, chemistry, and turbulence-chemistry interaction. The uncertainty in the established value of each parameter from these models affects the outcome of simulations. The important parameters for a turbulent simulation of a hydrogen-rich flame are determined using an adjoint-based sensitivity study. Then, the resultant uncertainty due to those parameters is determined with a Bayesian uncertainty framework.

Kalen Braman
Department of Aerospace Engr and Engr Mechanics
The University of Texas at Austin
kalen@utexas.edu

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

Venkat Raman, Robert D. Moser
University of Texas at Austin
v.raman@mail.utexas.edu, rmoser@ices.utexas.edu

MS9

Applications of Global Sensitivity Analysis to

Large Chemical-Kinetics Models and Beyond

It will be demonstrated how global sensitivity analysis can be used for chemical-kinetic model improvement and a detailed investigation of global sensitivity for the modeling of butanol oxidation will be presented, including an investigation of global sensitivity analysis for species. Extension to device modeling is introduced and future work on global sensitivity analysis for this case using sparse regression techniques will be discussed, along with some preliminary results. The talk reports on worked performed in collaboration with many researchers, particularly: Dingyu Zhou, Rex Skodje, Wei Liu, Raghu Sivaramakrishnan, Sibendu Som, and Douglas Longman.

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

MS9

A Stochastic Flamelet Model for Reactive Flow Computations Under Uncertainty

Abstract not available at time of publication.

Gianluca Iaccarino
Stanford University
Mechanical Engineering
jops@stanford.edu

MS9

Inference-based Assessment of Ab Initio Rate Coefficient Calculations

Ab initio methods to calculate rate coefficients are widely used in elementary kinetics research, yet the associated uncertainties are largely unexplored in a systematic manner. Here we focus on several simple H-abstraction reactions to study the types and magnitudes of variations in the calculated rate coefficients when various high-level electronic structure methods are used. The main sources of uncertainties are identified, and Bayesian inference is employed in conjunction with experimental data.

Jens Prager
Sandia National Laboratories
jens.prager@gmail.com

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

Ewa Papajak, Judit Zador
Sandia National Laboratories
epapaja@sandia.gov, jzador@sandia.gov

MS10

Virtual Dynamic Simulation of a Coal Fired Power Plant

Todays coal fired power plants require effective operation of large, highly integrated, multipurpose power and process systems. Virtual System Simulation is a vital tool for power station operators in order to give accurate, dynamic predictions of transient plant performance in real-time. Through such models it is possible to investigate the integration of new equipment, or the assessment and optimisation of overall plant performance through sensitivity studies and address technical barriers across power plant lifecycle-process innovation, design, operations, and management. However In general, full plant models and simulation tools are very fast and as a result their generality and accuracy can become compromised, as they are often fine-tuned to specific environments. Recently attempts were made to accurately simulate virtual coal-fired power plants by the authors. Integrated models incorporating both process simulation and CFD techniques provided an opportunity to take advantage of the benefits of both process simulation and detailed CFD modelling. The linkage of models generated in different commercial and/or proprietary software packages is becoming the state-of-the-art for the investigation of power generation applications. The integrated CFD-process models were applied successfully to conventional coal fired power generation applications showed an integrated CFD-process model of a pf combustion plant to compare well to experimental data from a 550 MWe power plant unit.

M Pourkashanian
Leeds University
m.pourkashanian@leeds.ac.uk

MS10

From Descriptive to Predictive and Back Again: The Need for Both Fundamental and Empirical Models in Coal Gasification

Coal combustion and gasification models have progressed from empiricism toward increasingly fundamental physical models. These can reveal underlying mechanisms, because these models get closer to reality - but at a higher cost. They are prohibitively expensive for practical scales. Expensive, highly resolved models can synthesize knowledge by informing reduced order and empirical models informing experimental campaigns. A synergy between simulation and experiments thus emerges. Concepts are illustrated with examples of entrained flow & in-situ multiphysics gasification simulators.

Charles Reid
Lawrence Livermore National Laboratories (LLNL)
reid24@llnl.gov

John Nitao
Lawrence Livermore Nat'l Lab
nitao1@llnl.gov

Julio Friedmann, David Camp
Lawrence Livermore National Laboratory
friedmann2@llnl.gov, camp2@llnl.gov

Philip Smith
University of Utah
philip.j.smith@gmail.com

MS10

A Comparative Study of Large Eddy Simulations of a Pulverised Coal Jet Flame

Large eddy simulations (LES) of a laboratory-scale piloted coal jet burner are carried out to study fundamental aspects of pulverised coal combustion (PCC). Three research groups at Freiberg, Duisburg and Stuttgart university use different codes, yet attempt to unify their comprehensive PCC models to study the flame. Non-reacting LES are in

good agreement with experimental evidence, while predictions of the reacting case show notable differences, highlighting the need for detailed PCC sub-model validation

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

Gregor Olenik
Stuttgart University
g.olenik@itv.uni-stuttgart.de

Andreas Kronenburg
Stuttgart University
Institute for Combustion Technology
kronenburg@itv.uni-stuttgart.de

Marco Ghiani
TU Freiberg
marco.ghiani@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

Mario Franchetti, Fabrizio Cavallo Marincola
Imperial College London
mario.franchetti05@imperial.ac.uk,
f.cavallo-marincola09@imperial.ac.uk

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

MS10

Large-Eddy Simulation of a Pulverized Coal Combustion Field in a Furnace with a Realistic Strong Swirling Burner

Large-eddy simulation (LES) is applied to a pulverized coal combustion field in a 100 kg/h scale test furnace with a realistic strong swirling burner to investigate fundamental characteristics of char combustion and, NOx and hydrogen sulfide formation. Three-dimensional unstructured LES code, named FrontFlowRed extended by CRIEPI, Kyoto University and NuFD is used. Results show that the present LES is capable of capturing the general feature of coal combustion behavior and the effects of combustion conditions.

Hiroaki Watanabe, Kenji Tanno
Central Research Institute of Electric Power Industry
CRIEPI
whiroaki@criepi.denken.or.jp, k-tanno@criepi.denken.or.jp

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

MS11

A ODT-Based Multiscale Framework for Turbulent Combustion Modeling

A multiscale modeling framework for turbulent combustion is presented. The framework couples large-eddy simulation (LES) with fine-grained one-dimensional turbulence (ODT). The 1D ODT solutions are embedded in LES and solve for the principal components; while, the LES solves for the flow. Two strategies for coupling LES and ODT are presented based on Eulerian and Lagrangian (flame-embedding) formulations. Results from the two LES-ODT formulations illustrate their potential to capture important non-equilibrium effects in combustion.

Tarek Echekki
North Carolina State University
techekk@eos.ncsu.edu

MS11

One-dimensional Turbulence Simulation: Advances and Application to Multi-phase Combustion

The one-dimensional turbulence model (ODT) is able to capture all scales of turbulent combustion, though in one dimension with modeling of large scales. Recent progress and advances in ODT research are presented. In addition, a multiphase ODT formulation is presented for solid particle combustion. Results of time-temperature statistics in particle flows with application to biological agent deactivation, along with flame propagation in biomass fuel beds with application to fire spread are presented.

David O. Lignell
Brigham Young University
davidlignell@byu.edu

John C. Hewson
Sandia National Laboratories
jchewso@sandia.gov

Guangyuan Sun, Abinash Paudel
Brigham Young University
gysungrad@gmail.com, abinashpaudel@gmail.com

MS11

The Contributions of LEM and ODT Toward a Better Understanding of Turbulent Flame Speeds

Abstract not available at time of publication.

Heiko Schmidt
BTU Cottbus
Mechanical Engineering
schmidth@tu-cottbus.de

MS11

One-Dimensional Turbulence: An Evaluation based on Comparisons with DNS Data for Turbulent Combustion

This talk presents comparisons of the ODT model to DNS data of nonpremixed and premixed flames. The calculations are done with an "Eulerian" variant of the originally proposed ODT model which allows direct comparisons with the DNS data. Initial conditions for ODT are extracted directly from the DNS and the same models for transport coefficients and chemical kinetics are employed. Based on the

results of these comparisons, the strengths and limitations of the model are discussed. Finally, a modeling technique is proposed that is based on ODT but overcomes many of the key limitations associated with ODT.

James C. Sutherland
University of Utah
James.Sutherland@utah.edu

MS12

Comparative Analysis of Uncertainties Associated with Transport and Chemical Kinetics in Laminar Flames

The relative importance of chemical kinetic and binary diffusion coefficients uncertainties is assessed in two key laminar flame configurations, namely: i) premixed flames and ii) non-premixed counterflow flames. Realistic uncertainties of selected active parameters were propagated in the target property space by using a Monte Carlo based High-Dimensional Model Representation. Results of characteristic flame properties suggest that, especially at high-pressure conditions, the propagated uncertainty of target properties due to binary diffusion coefficients is much smaller than the uncertainty due to chemical parameters.

Gaetano Esposito, Harsha Chelliah
University of Virginia
gaetano@virginia.edu, harsha@virginia.edu

MS12

Estimating and Utilizing Uncertainties in Theoretically Predicted Rate Coefficients

Various aspects of the uncertainties in theoretical kinetics predictions will be discussed. First, we will summarize the uncertainties in the components of ab initio transition state theory predictions for microcanonical rate coefficients. An illustration of the coupling of these uncertainties to yield overall uncertainties in the thermal kinetics will then be provided. Finally, we will discuss the utility of these uncertainties in a multiscale procedure for obtaining high-accuracy, self-consistent data for kinetic modeling.

Stephen Klippenstein, C. Franklin Goldsmith, Michael P. Burke
Argonne National Laboratory
sjk@anl.gov, franklin.goldsmith@gmail.com, mpburke@anl.gov

Alison S. Tomlin
Leeds University
a.s.tomlin@leeds.ac.uk

Lawrence B. Harding
Argonne National Laboratory
harding@anl.gov

MS12

Parameter Estimation with Missing Data

Uncertainty quantification on model predictions, using probabilistic methods, requires a full probabilistic specification, e.g. the joint density, for model parameters. Most commonly, only limited information, such as nominal values and error bards is available on model parameters or relevant data. In this talk, I will discuss means for handling this situation, to allow construction of a joint density on model parameters that is consistent with available information, in the absence of raw data. The method will be illustrated in the context of estimation of the joint density on Arrhenius chemical rate coefficients.

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

Cosmin Safta, Khachik Sargsyan
Sandia National Laboratories
csafta@sandia.gov, ksargsy@sandia.gov

Bert J. Debusschere
Energy Transportation Center
Sandia National Laboratories, Livermore CA
bjdebus@sandia.gov

Kenny Chowdhary
Sandia National Laboratories
kchowdh@sandia.gov

MS12

Deterministic Uncertainty Quantification Using Rational-quadratic Surrogate Models: Response Surface Modeling and Inference

Abstract not available at time of publication.

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