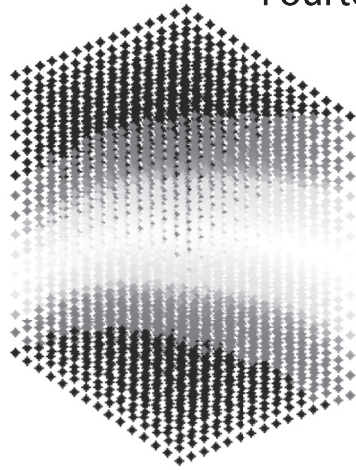


Final Program and Abstracts

Fourteenth International Conference on

Figure courtesy J. Breidt, T. Butler and D. Estep, SINUM Vol. 49, No. 5



NUMERICAL COMBUSTION

April 8-10, 2013

Holiday Inn San Antonio - Riverwalk
San Antonio, Texas, USA

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The SIAM registration desk is located in the Pre-function Area on the 7th floor. It is open during the following hours:

Sunday, April 7
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Tuesday, April 9
7:30 AM - 1:30 PM

Wednesday, April 10
7:30 AM - 4:00 PM

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NC13 Program-at-a-Glance

A Quick Guide to the 14th International Conference on Numerical Combustion

Key to abbreviations and symbols

-  = Coffee Break
-  = Refreshments Served
- CP = Contributed Presentation
- IP = Invited Plenary Speaker
- MS = Minisymposium
- * = Extended Session

NC13 At-a-Glance

Sunday
April 7

5:00 PM - 8:00 PM

Registration
Pre-function Area

6:00 PM - 8:00 PM

Welcome Reception
Skyline Atrium



Monday, April 8

7:00 AM - 4:00 PM

Registration
Pre-function Area

7:30 AM

Continental Breakfast
Skyline Atrium



8:00 AM - 8:15 AM

Welcoming Remarks
Tango 1 and 2

8:15 AM - 9:00 AM

IP1 Low Mach Number Simulation of Turbulent Combustion
John B. Bell, Lawrence Berkeley National Laboratory, USA
Tango 1 and 2

9:00 AM - 9:30 AM

Coffee Break
Skyline Atrium



9:30 AM - 11:30 AM

Concurrent Sessions

CP1 Complex Fuels

Tango 1

CP2 Engines

Tango 2

CP3 Numerical Methods I

Tango 4

CP4 Turbulence Modeling

Tango 3

11:30 AM - 1:00 PM

Lunch Break
Attendees on their own

1:00 PM - 3:00 PM

Concurrent Sessions

MS1 Uncertainty Quantification in Numerical Combustion - Part I of IV
Tango 1

MS2 Identification of State-Space Manifolds in Turbulent Combustion
Tango 2

CP5 Diffusion Controlled Non-Ideal Combustion

Tango 3

CP6 Jet Flames

Tango 4

CP7 LES I

Rumba

3:00 PM - 3:30 PM

Monday
April 8

Coffee Break
Skyline Atrium



3:30 PM - 5:30 PM

Concurrent Sessions

MS3 Uncertainty Quantification in Numerical Combustion - Part II of IV

Tango 1

***MS4** Detonation Dynamics and Structure - Part I of II

Tango 2

CP8 Sprays and Liquid Injection

Tango 4

CP9 Flamelets I

Rumba

CP10 Laminar Flames I

Tango 3

Tuesday, April 9

7:30 AM - 1:30 PM

Registration
Pre-function Area

7:30 AM

Continental Breakfast
Skyline Atrium



8:10 AM - 8:15 AM

Remarks
Tango 1 and 2

8:15 AM - 9:00 AM

IP2 Multi-scale Analysis Tools in Reacting Flows
Dimitris Goussis, National Technical University of Athens, Greece
Tango 1 and 2

9:00 AM - 9:30 AM

Coffee Break
Skyline Atrium



9:30 AM - 11:30 AM

Concurrent Sessions

MS5 Multi-Discipline Advances in Combustion Tubes

Tango 1

MS6 Coal Combustion and Gasification: From Fundamental Processes to Technical Applications - Part I of II
Tango 2

CP11 LES II

Rumba

CP12 Numerical Methods II

Tango 4

CP13 Soot and Particulates

Tango 3

Tuesday
April 9

11:30 AM - 1:00 PM

Lunch Break
Attendees on their own

1:00 PM - 3:00 PM

Concurrent Sessions

MS7 Detonation Dynamics and Structure - Part II of II
Tango 2

MS8 Hybrid CPU+Accelerator Simulation Techniques for Reacting Flows with Complex Chemical Kinetics
Tango 1

CP14 Topological and Geometrical Modeling of Flames
Tango 3

CP15 Detailed and Reduced Chemistry
Tango 4

CP16 Direct Numerical Simulation
Rumba

3:00 PM

Sessions Conclude for Attendees to Explore San Antonio

Wednesday, April 10

7:30 AM - 4:00 PM

Registration
Pre-function Area

7:30 AM

Continental Breakfast
Skyline Atrium



8:10 AM - 8:15 AM

Closing Remarks
Tango 1 and 2

8:15 AM - 9:00 AM

IP3 Numerical Modeling of Pollutant Emissions with Detailed Kinetics: from Ideal Reactors to Flames
Tiziano Faravelli, Politecnico di Milano, Italy
Tango 1 and 2

9:00 AM - 9:30 AM

Coffee Break
Skyline Atrium



9:30 AM - 11:30 AM

Concurrent Sessions

MS9 Uncertainty Quantification in Numerical Combustion - Part III of IV

Tango 1

CP17 Bio-Mass/Coal

Tango 2

CP18 Compressible Reacting Flow

Rumba

CP19 Laminar Flames II

Wednesday
April 10

Tango 3

CP20 Numerical Methods III
Tango 4

11:30 AM - 1:00 PM

Lunch Break
Attendees on their own

1:00 PM - 3:00 PM

Concurrent Sessions

MS10 Coal Combustion and Gasification: From Fundamental Processes to Technical Applications - Part II of II
Tango 2

CP21 Detonation I

Tango 4

CP22 LES III

Rumba

CP23 Stability

Tango 1

CP24 Statistical and PDF Methods
Tango 3

3:00 PM - 3:30 PM

Coffee Break
Skyline Atrium



3:30 PM - 5:30 PM

Concurrent Sessions

MS11 Applications and Advances in One-dimensional Turbulence Simulation

Tango 2

MS12 Uncertainty Quantification in Numerical Combustion - Part IV of IV

Tango 1

CP25 Detonation II

Tango 4

CP26 Flamelets II

Rumba

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- Welcome Reception

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April 10.

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Sven Leyffer, SIAM Vice President for Programs (vpp@siam.org)

Get-together

- Welcome Reception
Sunday, April 7
6:00-8:00 PM



Rio San Antonio Cruises

Sessions will end early on Tuesday, April 9, to allow attendees the opportunity to explore the local area or to take a River Boat Tour. The River Boat Tour is a 35 to 40 minute, non-stop, narrated tour. Boats depart various locations along the River Walk every 15 to 20 minutes. If you did not purchase a discounted ticket during the pre-registration process, you may purchase a regular rate ticket through Rio San Antonio Cruises (http://www.riosanantonio.com/?page_id=2).

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Invited Plenary Speakers

**** All Invited Plenary Presentations will take place in Tango 1 and 2****

Monday, April 8

8:15 AM - 9:00 AM

IP1 Low Mach Number Simulation of Turbulent Combustion

John B. Bell, *Lawrence Berkeley National Laboratory, USA*

Tuesday, April 9

8:15 AM - 9:00 AM

IP2 Multi-scale Analysis Tools in Reacting Flows

Dimitris Goussis, *National Technical University of Athens, Greece*

Wednesday, April 10

8:15 AM - 9:00 AM

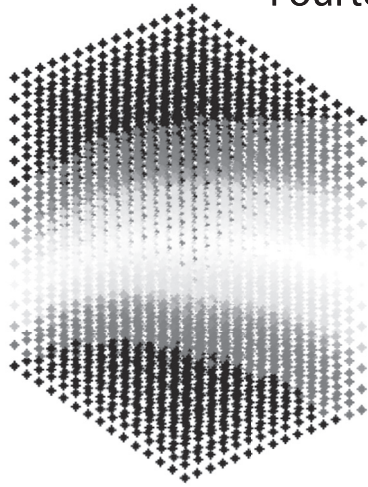
IP3 Numerical Modeling of Pollutant Emissions with Detailed Kinetics:
from Ideal Reactors to Flames

Tiziano Faravelli, *Politecnico di Milano, Italy*

Notes

NC13 Program

Fourteenth International Conference on



NUMERICAL COMBUSTION

April 8-10, 2013

Holiday Inn San Antonio - Riverwalk
San Antonio, Texas, USA

Figure courtesy J. Breidt, T. Butler and D. Estep, SINUM Vol. 49, No. 5

Sunday, April 7

Registration

5:00 PM-8:00 PM

Room: Pre-function Area

Welcome Reception

6:00 PM-8:00 PM

Room: Skyline Atrium



Monday, April 8

Registration

7:00 AM-4:00 PM

Room: Pre-function Area

Continental Breakfast

7:30 AM

Room: Skyline Atrium



Welcoming Remarks

8:00 AM-8:15 AM

Room: Tango 1 and 2

IP1

Low Mach Number Simulation of Turbulent Combustion

8:15 AM-9:00 AM

Room: Tango 1 and 2

Chair: Mitchell Smooke, Yale University, USA

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

Lawrence Berkeley National Laboratory, USA

Monday, April 8

Coffee Break

9:00 AM-9:30 AM



Room: Skyline Atrium

CP1

Complex Fuels

9:30 AM-10:50 AM

Room: Tango 1

Chair: Constandinos Mitsingas, University of Illinois at Urbana-Champaign, USA

9:30-9:45 Kinetic Modeling Study of the Oxidation of Larger Methylated Hydrocarbons

Marileen L. Fischer, Elke Goos, and Uwe Riedel, German Aerospace Center, Stuttgart, Germany

9:50-10:05 Simulation of Refinery Gas Composition Effect on Physicochemical Properties of Combustion Products

Lourdes I. Merino and Oscar Cala, Universidad Industrial de Santander, Colombia; Jaqueline Saavedra, Instituto Colombiano del Petroleo, Colombia; Viatcheslav Kafarov, Universidad Industrial de Santander, Colombia

10:10-10:25 Extinction Strain Rate Simulations for Three Butanol Isomers

Constandinos M. Mitsingas and Dimitrios Kyritsis, University of Illinois at Urbana-Champaign, USA

10:30-10:45 Revisiting the Shrinking-Core Model of Sub-Micron Aluminum Combustion

John D. Buckmaster, Buckmaster Research, USA; Thomas Jackson, University of Illinois at Urbana-Champaign, USA

Monday, April 8

CP2

Engines

9:30 AM-11:30 AM

Room: Tango 2

Chair: Jonathan D. Regele, Iowa State University, USA

9:30-9:45 Direct Numerical Simulations of HCCI and SACI with Ethanol

Ankit Bhagatwala and Jacqueline Chen, Sandia National Laboratories, USA

9:50-10:05 Numerical Investigations of Combustion Regimes for Dual-Fuel Engines Applications

Stephane Jay, Haïfa Belaïd-Saleh and Cécile Pera, IFP Energies Nouvelles, France

10:10-10:25 Modeling of RCCI Combustion

Ulas Eguz and Bart Somers, Eindhoven University of Technology, Netherlands; Philip de Goeij, Technische Universiteit Eindhoven, The Netherlands

10:30-10:45 Acoustic Timescale Characterization of Diffusion-Free Unreacted Pocket Ignition

Jonathan D. Regele, Iowa State University, USA

10:50-11:05 Hydrogen-Air Mixing Layer Ignition at Temperatures below Crossover

Eduardo Fernandez-Tarrazo and Antonio Sánchez, Universidad Carlos III de Madrid, Spain; Amable Liñán, Universidad Politécnica de Madrid, Spain; Forman Williams, University of California, San Diego, USA

11:10-11:25 Ready - a Reactive Dynamic Simulation for Hydrogen Combustion

César Mogo and João Brandão, Universidade do Algarve, Portugal

Monday, April 8

CP3

Numerical Methods I

9:30 AM-11:30 AM

Room: Tango 4

Chair: Matthias Ihme, Stanford University, USA

9:30-9:45 An Adaptive Deferred Correction Coupling Strategy for Low Mach Number Flows with Detailed Chemistry and Transport

Marc Day, Andrew Nonaka, and John B. Bell, Lawrence Berkeley National Laboratory, USA

9:50-10:05 Local Rectangular Refinement in Three Dimensions (LRR3D) with Application to Unsteady Combustion Problems

Beth Anne V. Bennett and Mitchell Smooke, Yale University, USA

10:10-10:25 Parallel Implicit Adaptive Mesh Refinement Scheme for Unsteady Laminar Reactive Flows

Clinton P. Groth, and Scott Northrup, University of Toronto, Canada

10:30-10:45 A Robust Multigrid Method for Turbulent, Chemically Reacting Flows

Mark Wasserman, Technion - Israel Institute of Technology, Israel; Yair Mor-Yossef, Israeli CFD Center, Israel; Barry Greenberg, Technion - Israel Institute of Technology, Israel

10:50-11:05 High-Order CENO Finite-Volume Scheme for Large-Eddy Simulation of Turbulent Premixed Flames

Marc R. Charest, and Clinton P. Groth, University of Toronto, Canada; Pierre Gauthier, Rolls-Royce Canada Limited, Canada

11:10-11:25 An Implicit-Compact Method for the Investigation of Time-Dependent Laminar Flames

Richard Dobbins and Mitchell Smooke, Yale University, USA

Monday, April 8

CP4

Turbulence Modeling

9:30 AM-11:30 AM

Room: Tango 3

Chair: Alan Kerstein, Sandia National Laboratories, USA

9:30-9:45 Sub-Grid Modelling of Non-Premixed Turbulent Flames

Salvador Navarro-Martinez, Imperial College London, United Kingdom

9:50-10:05 Extinction and Reignition in Turbulent Nonpremixed Jet Flames with Vitiated Coflow: a One-Dimensional-Turbulence Study

Esteban Gonzalez, Combustion Science and Engineering, Inc., USA; David O. Lignell, Brigham Young University, USA; Ponnuthurai Gokulakrishnan and Michael Klassen, Combustion Science and Engineering, Inc., USA

10:10-10:25 Studying the Impact of Shear onto the Mixing Processes of a Turbulent Stratified Flame by Means of Large Eddy Simulation

Amer Avdic, Guido Kuenne, Anja Ketelheun, Amsini Sadiki, and Johannes Janicka, Technische Universität Darmstadt, Germany

10:30-10:45 Extinction Phenomena in Highly Turbulent Premixed Counterflow Flames

Sgouria Lyra, Hemanth Kolla, Bruno Coriton, Jonathan Frank, Janine Bennett, and Jacqueline Chen, Sandia National Laboratories, USA

10:50-11:05 Effects of Turbulent Reynolds Number on Turbulent Scalar Flux Transport in Premixed Flames

Robert S. Cant, University of Cambridge, United Kingdom; Nilanjan Chakraborty, Newcastle University, United Kingdom

11:10-11:25 Influence of Gas Expansion on Premixed Flame Flashback in Turbulent Channel Flow

Damir M. Valiev, Sandia National Laboratories, USA; Andrea Gruber, SINTEF Energy Research, Norway; Hemanth Kolla and Jacqueline H. Chen, Sandia National Laboratories, USA; Chung K. Law, Princeton University, USA

Lunch Break

11:30 AM-1:00 PM

Attendees on their own

Monday, April 8

MS1

Uncertainty Quantification in Numerical Combustion - Part I of IV

1:00 PM-3:00 PM

Room: Tango 1

For Part 2 see MS3

Chemically reacting flow models involve a large number of parameters, which are typically estimated from experiments or computations. Quantifying uncertainties in these parameters, and associated computational predictions, is necessary for assessment of predictability in combustion models, for model selection and validation, and for enabling decision support. This minisymposium explores a wide range of topics in uncertainty quantification with particular focus on their application in computational reacting flow.

Organizer: Habib N. Najm
Sandia National Laboratories, USA

1:00-1:25 Understanding and Simplifying Chemical Processes Using Markov Chains

Luca Tosatto and Youssef M. Marzouk,
Massachusetts Institute of Technology, USA

1:30-1:55 Reaction Pathway Analysis Using Stochastic Sampling

Rex Skodje, University of Colorado Boulder, USA

2:00-2:25 Uncertainty Quantification Applied to Combustion Experiment Design

Hai Wang, University of Southern California, USA

2:30-2:55 Determination of the Uncertainty of Reaction Rate Parameters

Tamas Turanyi, Eötvös University, Hungary

Monday, April 8

MS2

Identification of State-Space Manifolds in Turbulent Combustion

1:00 PM-3:00 PM

Room: Tango 2

Manifolds are widely recognized to be present in combustion processes. As the overlap of mixing and reaction timescales increases, the dimensionality of these manifolds also increases. Traditional methods of parameterizing the state-space for, e.g. nonpremixed combustion rely on a-priori postulation of the controlling variables (the steady laminar flamelet model is an example). This minisymposium explores a few methodologies that seek to identify and exploit these manifolds. Additionally, identification of the dimensionality of a manifold required to obtain a desired accuracy will be covered.

Organizer: James C. Sutherland
University of Utah, USA

Organizer: Alessandro Parente
Université Libre de Bruxelles, Belgium

1:00-1:25 Development of Reduced Order Models Based on Principal Components and Principal Variables

Alessandro Parente, University of Pisa, Italy; James C. Sutherland, University of Utah, USA; Ben Isaac, University of Utah, USA & Université Libre de Bruxelles, Belgium

1:30-1:55 PCA-Based Parameterization of Composition Space in Turbulent Combustion and Implications to Modeling

Tarek Echehki, North Carolina State University, USA

2:00-2:25 The Identification and Use of Empirical Manifolds in Turbulent Combustion

Stephen B. Pope and Yue Yang, Cornell University, USA

2:30-2:55 Tabulation of Diluted Flamelets for MILD Combustion Modelling

Jean Lamouroux, Ecole Centrale Paris, France; Matthias Ihme, Stanford University, USA; Benoit Fiorina, First Nasser Darabiha, and Olivier Gicquel, Ecole Centrale Paris, France

Monday, April 8

CP5

Diffusion Controlled Non-Ideal Combustion

1:00 PM-2:40 PM

Room: Tango 3

Chair: Stewart Cant, University of Cambridge, United Kingdom

1:00-1:15 CFD Modeling of Radiation Effects in a Partial Oxidation Flame Including Optically Thin and Dense Regions

Franziska Hunger, Bjoern Stelzner, Dimosthenis Trimis, and Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

1:20-1:35 Preferential Diffusion in Bluff-Body Stabilized Turbulent Premixed Flames

Viswanath R. Katta, Innovative Scientific Solution, USA; William Roquemore, Air Force Research Laboratory, USA

1:40-1:55 Nonideal Diffusion in Supercritical Flows

Pierre Gaillard, ONERA, France; Vincent Giovangigli, CMAP, Ecole Polytechnique, France; Lionel Matuszewski, ONERA, France

2:00-2:15 A New Methodology to Incorporate Differential Diffusion in Cfd Simulations of Reactive Flows

Georgios Maragkos, Pieter Rauwoens, and Bart Merci, Ghent University, Belgium

2:20-2:35 Numerical Modeling of Multiphase Multicomponent Combustion in the Titanium-Boron System

Sushil Kumar P. Koundinyan, John Bdzil, Moshe Matalon, and D. Scott Stewart, University of Illinois at Urbana-Champaign, USA

Monday, April 8

CP6

Jet Flames

1:00 PM-3:00 PM

Room: Tango 4

Chair: Forman Williams, University of California, San Diego, USA

1:00-1:15 Direct Numerical Simulation of the Stabilization Mechanism of a Turbulent Reacting Hydrogen Jet in Supersonic Cross-Flow

Amirreza Saghaffian, Stanford University, USA; Heinz Pitsch, RWTH Aachen University, Germany

1:20-1:35 Conditional Moment Closure Modeling of Differential Diffusion in A Turbulent Hydrogen Jet Flame

Dominic Ma and Cecile B. Devaud, University of Waterloo, Canada

1:40-1:55 Rans Simulation of a Confined Turbulent Jet Diffusion Flame Using Conditional Source-Term Estimation

Jeffrey Labahn and Cecile B. Devaud, University of Waterloo, Canada

2:00-2:15 Influence of Boundary Layer Trip on Non-Swirling and Swirling Reacting Jets Using Large Eddy Simulation

Soufien Taamallah, Konstantina Vogiatzaki, Gaurav Kewlani, Santosh Shanbhogue, and Ahmed F Ghoniem, Massachusetts Institute of Technology, USA

2:20-2:35 Characterization of Ignition and Stabilization Mechanisms of a Pulsating Jet Flame

Yuntao Chen, University of Michigan, Ann Arbor, USA; Matthias Ihme, Stanford University, USA

2:40-2:55 Dns of Soot Formation in Three Dimensional Turbulent Non-Premixed Jet Flames

Antonio Attili and Fabrizio Bisetti, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Michael E. Mueller, Princeton University, USA; Heinz Pitsch, RWTH Aachen University, Germany

Monday, April 8

CP7

LES I

1:00 PM-3:00 PM

Room: Rumba

Chair: Dan Haworth, Pennsylvania State University, USA

1:00-1:15 Les of a Premixed Jet Flame at Intense Turbulence

Philipp Trisjono, RWTH Aachen University, Germany; Obulescu Chatakonda, University of New South Wales, Australia; Heinz Pitsch, RWTH Aachen University, Germany; Evatt R. Hawkes, University of New South Wales, Australia; Jacqueline Chen, Sandia National Laboratories, USA

1:20-1:35 The Impact of a Les Combustion Model on the Prediction of Flame Dynamics

Benoit Fiorina, Pierre Auzillon, Olivier Gicquel, and Denis Veynante, Ecole Centrale Paris, France

1:40-1:55 Large Eddy Simulation of Premixed Combustion Using Conditional Source-Term Estimation for Complex Geometries

Girish V. Nivarti, M. Mahdi Salehi, and W. Kendal Bushe, University of British Columbia, Canada

2:00-2:15 Large Eddy Simulation of Swirl Stabilized Lean Premixed Combustion Using Structured and Unstructured Solvers

Guido Kuenne, Kai Aschmoneit, Anja Ketelheun, and Johannes Janicka, Technische Universität Darmstadt, Germany

2:20-2:35 Les/dns Modelling of Mesocombustion Chambers with Arrhenius Complex Chemistry

Pierre Benard, Vincent Moureau, Yves D'Angelo, Ghislain Lartigue, and Marianne Cuif-Sjöstrand, CORIA, France

2:40-2:55 Large Eddy Simulation of Turbulent Non-Premixed Flames Using Conditional Source-Term Estimation

Graham R. Hendra, Kendal Bushe, and M. Mahdi Salehi, University of British Columbia, Canada

Coffee Break

3:00 PM-3:30 PM

Room: Skyline Atrium



Monday, April 8

MS3

Uncertainty Quantification in Numerical Combustion - Part II of IV

3:30 PM-5:30 PM

Room: Tango 1

For Part 1 see MS1

For Part 3 see MS9

Chemically reacting flow models involve a large number of parameters, which are typically estimated from experiments or computations. Quantifying uncertainties in these parameters, and associated computational predictions, is necessary for assessment of predictability in combustion models, for model selection and validation, and for enabling decision support. This minisymposium explores a wide range of topics in uncertainty quantification with particular focus on their application in computational reacting flow.

Organizer: Habib N. Najm
Sandia National Laboratories, USA

3:30-3:55 Enforcing Positivity in Intrusive PC-UQ Methods for Reactive ODEs Systems

Mauro Valorani, Università di Roma "La Sapienza", Italy; Habib N. Najm, Sandia National Laboratories, USA

4:00-4:25 Quantifying Uncertainty of Ion Chemistry in Premixed Methane-air Flames

Francesco Rizzi, Duke University, USA; Mbark El Morsli and Fabrizio Bisetti, King Abdullah University of Science & Technology (KAUST), Saudi Arabia; Omar M. Knio, Duke University, USA

4:30-4:55 Hierarchical Validation & Uncertainty Quantification of Flare Combustion Efficiency with Large Eddy Simulations

Philip J. Smith, Sean Smith, Jeremy Thornock, and Anchal Jatale, University of Utah, USA

5:00-5:25 Chemical Kinetic Model Development Using Bayesian Variable Selection

Nikhil Galagali and Youssef M. Marzouk, Massachusetts Institute of Technology, USA

Monday, April 8

MS4

Detonation Dynamics and Structure - Part I of II

3:30 PM-6:00 PM

Room: Tango 2

For Part 2 see MS7

The accurate description of detonation evolution and structure in homogeneous and heterogeneous reactive media remains a significant challenge and a topic of ongoing research. Mathematical models typically involve nonlinear PDEs supplemented by non-ideal equations of state and stiff source terms. When reaction is strongly state-sensitive, instabilities are the norm and chemico-hydrodynamic coupling generates complex, unsteady structures. For heterogeneous explosives, or when the confining walls are compliant, accurate numerical treatment of multi-material and multi-phase models is an additional requirement. The talks will focus on adaptive, high-order numerical methods and well-resolved numerical results for a variety of problems including detonation initiation, stability, reflection, diffraction, response to confinement, and failure.

Organizer: Donald W. Schwendeman

Rensselaer Polytechnic Institute, USA

Organizer: Ashwani K. Kapila
Rensselaer Polytechnic Institute, USA

3:30-3:55 Shock-induced Cavity Collapse with Reaction

Donald W. Schwendeman and Ashwani K. Kapila, Rensselaer Polytechnic Institute, USA

4:00-4:25 Some Advances on Numerical Methods for Hyperbolic Balance Laws and Applications

Eleuterio F. Toro, University of Trento, Italy

4:30-4:55 Heterogeneous Nitromethane Ignition and Transition to Detonation

Louisa Michael and Nikos Nikiforakis, University of Cambridge, United Kingdom

continued in next column

5:00-5:25 Cavity Collapse in Elastic-plastic Materials

Elizabeth R. Johnstone and Nikos Nikiforakis, University of Cambridge, United Kingdom

5:30-5:55 Multi-phase Detonations in Elastic-plastic Confinement

Stefan Schoch and Nikos Nikiforakis, University of Cambridge, United Kingdom

Monday, April 8

CP8

Sprays and Liquid Injection

3:30 PM-5:10 PM

Room: Tango 4

Chair: Mazyar Jalaal, University of British Columbia, Canada

3:30-3:45 Modeling and Numerical Treatment of Liquid Injection Processes at High-Pressure Supercritical Conditions

Joseph C. Oefelein, Rainer Dahms, Guilhem Lacaze, and Anthony Ruiz, Sandia National Laboratories, USA

3:50-4:05 Fuel Injection: A Direct Numerical Simulation of Primary Atomization

Mazyar Jalaal and Kian Mehravaran, University of British Columbia, Canada

4:10-4:25 Modeling Aspects of Evaporative Fuel Scalar in Tabulated Chemistry Approach for Diesel Spray Combustion

Sridhar Ayyapureddi, Bart Somers, and Philip De Goey, Eindhoven University of Technology, Netherlands

4:30-4:45 Ignition of Fuel Sprays in Laminar Mixing Layers

Daniel Martínez-Ruiz, Universidad Carlos III de Madrid, Spain; Javier Urzay, Stanford University, USA; Antonio Sánchez, Universidad Carlos III de Madrid, Spain; Forman Williams, University of California, San Diego, USA

4:50-5:05 Influence of Fuel Staging on the Spray Characteristics in a Staged Multipoint Burner

Sebastien Ducruix, Laboratoire EM2C, France; Benoit Cheneau, SAFRAN, SNECMA, France

Monday, April 8

CP9**Flamelets I**

3:30 PM-5:30 PM

Room: Rumba

Chair: Yuan Xuan, California Institute of Technology, USA

3:30-3:45 Implementation of Soot Model in Flamelet Generated Manifold (FGM) for Spray H Conditions of ECN Database

Sridhar Ayyapureddi, Eindhoven University of Technology, Netherlands; Mariano Sirignano, Università Federico II, Italy; Bart Somers, Eindhoven University of Technology, Netherlands; D'Anna Andrea, Università Federico II, Italy; Philip De Goey, Eindhoven University of Technology, Netherlands

3:50-4:05 A Flamelet-Based Relaxation Model for Polycyclic Aromatic Hydrocarbons

Yuan Xuan, Pauline Vervisch-Kljakic, and Guillaume Blanquart, California Institute of Technology, USA

4:10-4:25 Flamelet Modeling of Radiation Effects in a Partial Oxidation Flame

Franziska Hunger, Danny Messig, and Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

4:30-4:45 Budget-Analysis and Model-Assessment of Unsteady Flamelet-Formulation

Wai Lee Chan, University of Michigan, Ann Arbor, USA; Matthias Ihme, Stanford University, USA; Hemanth Kolla and Jacqueline Chen, Sandia National Laboratories, USA

4:50-5:05 Numerical Investigation of Premixed Turbulent Flame Using Tabulated Filtered Flame (F-Tacles) Combustion Model

Arash Hossein Zadeh, Technische Universität Darmstadt, Germany; Thomas Schmitt, Ecole Centrale Paris, France; Amsini Sadiki and Johannes Janicka, Technische Universität Darmstadt, Germany

5:10-5:25 Flamelet Modeling of High Pressure Partial Oxidation

Danny Messig, Bernd Meyer, and Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

Monday, April 8

CP10**Laminar Flames I**

3:30 PM-5:10 PM

Room: Tango 3

Chair: Su Cao, Yale University, USA

3:30-3:45 Simulation of Premixed Flames Using Integral Reaction Zone Modelling

Christian Bruzzese and Andreas Class, Karlsruhe Institute of Technology, Germany

3:50-4:05 Numerical Modeling of Laminar, Reactive Flows with Detailed Kinetic Mechanisms

Alberto Cuoci, Alessio Frassoldati, Tiziano Faravelli, and Eliseo Ranzi, Politecnico di Milano, Italy

4:10-4:25 Simulations of Axisymmetric Coflow Laminar Diffusion Flames

Adhiraj K. Dasgupta, Somesh P. Roy, and Daniel C. Haworth, Pennsylvania State University, USA

4:30-4:45 Triple-Flame Propagation Against a Poiseuille Flow in a Porous Channel

Faisal A. Al-Malki, Taif University, Saudia Arabia; Joel Daou, University of Manchester, United Kingdom

4:50-5:05 Effects of Pressure and Fuel Stream Dilution on the Structure of Axisymmetric Coflow Methane-Air Laminar Diffusion Flames: A Computational and Experimental Study

Su Cao, Beth Anne V. Bennett, Bin Ma, Marshall Long, and Mitchell Smooke, Yale University, USA

Tuesday, April 9**Registration**

7:30 AM-1:30 PM

Room: Pre-function Area

Continental Breakfast

7:30 AM

Room: Skyline Atrium

Remarks

8:10 AM-8:15 AM

Room: Tango 1 and 2

IP2**Multi-scale Analysis Tools in Reacting Flows**

8:15 AM-9:00 AM

Room: Tango 1 and 2

Chair: D. Scott Stewart, University of Illinois at Urbana-Champaign, USA

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

Coffee Break

9:00 AM-9:30 AM

Room: Skyline Atrium



Tuesday, April 9

MS5

Multi-Discipline Advances in Combustion Tubes

9:30 AM-11:30 AM

Room: Tango 1

Combustion tubes have numerous applications – from thermopower waves in nanotubes till large-scale safety issues in subways and mines. This minisymposium is aimed to consolidate the entire multi-discipline knowledge, get rid of existing discrepancies between various approaches, and develop strategies for future works. The first speaker discusses various mechanisms of flame acceleration and deflagration-to-detonation transition such as that through finger flame shape, wall friction, and flame-obstacle interaction. An alternative mechanism, through hydraulic resistance, is presented by the second speaker. The third speaker shows the effect of viscous drag on flame propagation. Finally, the fourth speaker discusses the possibility of kinetics study.

Organizer: V'yacheslav Akkerman
West Virginia University, USA

Organizer: Kaoru Maruta
Tohoku University, Japan

9:30-9:55 On Flame Acceleration and Deflagration-to-Detonation Transition in Tubes

V'yacheslav Akkerman, West Virginia University, USA; Vitaly Bychkov, Umeå University, Sweden; Chung K. Law, Princeton University, USA; Damir M. Valiev, Sandia National Laboratories, USA

10:00-10:25 On Numerical Analysis of Hydraulic Resistance Phenomena in Obstructed Channels

Viatcheslav Bykov, Mikhail Kuznetsov, and Jorge Yanez, Karlsruhe Institute of Technology, Germany

10:30-10:55 Flame Dynamics in Long Open Channels

Vadim Kurdyumov, CIEMAT, Madrid, Spain; Moshe Matalon, University of Illinois at Urbana-Champaign, USA

continued in next column

11:00-11:25 Possibility of Kinetics Study in Tubes

Hisahi Nakamura, Takuya Tezuka, Susumu Hasegawa, and Kaoru Maruta, Tohoku University, Japan

Tuesday, April 9

MS6

Coal Combustion and Gasification: From Fundamental Processes to Technical Applications - Part I of II

9:30 AM-11:30 AM

Room: Tango 2

For Part 2 see MS10

Coal combustion and gasification are still the dominating processes to generate electrical base load power and chemical feedstocks. Further optimization of these high temperature conversion processes heavily relies on numerical modeling. CFD of thermal coal conversion requires reliable sub-models to account for turbulence, particle transport, pyrolysis, heterogeneous char reactions and homogeneous combustion. The first session focuses on recent sub-model developments. Also, needs for experimental benchmark data for model validation are presented. The second session focuses on CFD modeling. Target applications ranging from small laboratory flames to pilot scale furnaces are investigated looking at aspects such as coal flame structure and pollutant formation.

Organizer: Christian Hasse
Technische Universität Bergakademie Freiberg, Germany

Organizer: Oliver T. Stein
Universität Stuttgart, Germany

Organizer: Andres Kempf
University of Duisburg-Essen, Germany

9:30-9:55 Influence of Chemical Pyrolysis Product Composition on Coal Particle Ignition

Michele Vascellari, Technische Universität Bergakademie Freiberg, Germany; Rahul Arora, Indian Institute of Technology, Delhi, India; Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

10:00-10:25 The Role of Chemical Structure in Predictions of Coal Pyrolysis and Char Conversion

Tom Fletcher, Brigham Young University, USA

continued on next page

10:30-10:55 Managing Computational Chemistry for Gasification Modeling Through the C3M Software

Dirk Van Essendelft, Chris Guenther, and Mehrdad Shahnaim, National Energy Technology Laboratory, USA; Nathan Weiland, Richard Turton, and Kiran Chaudhari, West Virginia University, USA; Phil Nicoletti, Tingwen Li, Terry Jordan, and Justin Weber, National Energy Technology Laboratory, USA

11:00-11:25 Experimental Considerations in Providing Benchmark Data on Pulverized Coal Ignition and Char Particle Burning Rates

Christopher Shaddix, Sandia National Laboratories, USA

Tuesday, April 9

CP11

LES II

9:30 AM-11:30 AM

Room: Rumba

Chair: Heinz Pitsch, Stanford University, USA

9:30-9:45 Hybrid Transported-Tabulated Strategy to Downsize Detailed Chemistry for Large Eddy Simulation

Guillaume Ribert, INSA de Rouen, France; Pascale Domingo, CORIA, France; Luc Vervisch, INSA Rouen, France

9:50-10:05 Explicitly Filtered Large Eddy Simulation for Conserved Scalar Modeling of Turbulent Combustion

Colin Heye, University of Texas at Austin, USA; Colleen Kaul, Stanford University, USA; Venkat Raman, University of Texas at Austin, USA

10:10-10:25 Large Eddy Simulation of a Gas Turbine Model Combustor

Yee Chee See, University of Michigan, USA

10:30-10:45 Les of Natural Fire Propagation in a Lab-Scale Configuration

Melanie C. Rochoux, Benedicte Cuenot, and Eleonore Riber, CERFACS, France; Denis Veynante and Nasser Darabiha, Ecole Centrale Paris, France

10:50-11:05 Comparison of Inflow Generation Methods for LES of Turbulent Flames

Dirk Dietzel and Danny Messig, Technische Universität Bergakademie Freiberg, Germany; Federico Piscaglia and Andrea Montorfano, Politecnico di Milano, Italy; Gregor Olinek, Oliver T. Stein, and Andreas Kronenburg, Universität Stuttgart, Germany; Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

11:10-11:25 A Conditional Moment Closure Formulation for Large Eddy Simulation of Compressible Non-Premixed Turbulent Reactive Flows

Mauro Valorani, *Pietro Paolo Ciottoli*, Matteo Bernardini, and Sergio Pirozzoli, Università di Roma "La Sapienza", Italy

Tuesday, April 9

CP12

Numerical Methods II

9:30 AM-11:30 AM

Room: Tango 4

Chair: Beth Bennett, Yale University, USA

9:30-9:45 On-the-Fly Processing and Feature Extraction of Flame and Flow Properties Obtained by Direct Numerical Simulation

Timo Oster, Gordon Fru Atanga, Abouelmagd Abdelsamie, and Dominique Thévenin, University of Magdeburg, Germany

9:50-10:05 Implementation of Unsteady Plug Flow Reactors in Cantera

David W. Mikolaitis, University of Florida, USA

10:10-10:25 Time-Implicit Schemes with Multiresolution Adaptive Meshing for Combustion Fronts

Max Duarte, Richard Dobbins, and Mitchell Smooke, Yale University, USA

10:30-10:45 Ember: An Unsteady Quasi-1D Flame Solver

Raymond L. Speth and William H. Green, Massachusetts Institute of Technology, USA

10:50-11:05 Spurious Behavior of Shock-Capturing Methods: Problems Containing Stiff Source Terms & Discontinuities

Helen Yee, NASA Ames Research Center, USA; Dmitry Kotov, Stanford University, USA; Wei Wang, Florida International University, USA; Chi-Wang Shu, Brown University, USA

11:10-11:25 Interface Tracking of a Chemical Reacting Carbon Particle Moving in CO₂ Atmosphere

Frank Dierich and Petr Nikrityuk, Technische Universität Bergakademie Freiberg, Germany

Tuesday, April 9

CP13

Soot and Particulates

9:30 AM-11:30 AM

Room: Tango 3

Chair: Marc R. Charest, University of Toronto, Canada

9:30-9:45 A Computational Study of Turbulent Nonpremixed Sooting Flames Using a High Order Method of Moments

Paul Arias, University of Michigan, Ann Arbor, USA; Vivien Lecoustre, University of Maryland, USA; Somesh P. Roy, Pennsylvania State University, USA; Zhaoyu Luo, University of Connecticut, USA; Daniel C. Haworth, Pennsylvania State University, USA; Hong G. Im, University of Michigan, USA; Tianfeng Lu, University of Connecticut, USA; Kwan-Liu Ma, University of California, Davis, USA; Ramanan Sankaran, Oak Ridge National Laboratory, USA; Arnaud Trounev, University of Maryland, USA

9:50-10:05 The Contribution of Nucleation and Condensation to Soot Morphology

Nickolas A. Eaves and Murray Thomson, University of Toronto, Canada; Seth Dworkin, Ryerson University, Canada

10:10-10:25 An Assessment of Aerosol-Dynamics-Based Detailed Soot Models in Laminar Premixed Flames

Somesh P. Roy and Daniel C. Haworth, Pennsylvania State University, USA

10:30-10:45 Effects of Turbulent Combustion Modeling Errors on Soot Evolution in Turbulent Nonpremixed Jet Flames

Michael E. Mueller, Princeton University, USA; Venkat Raman, University of Texas at Austin, USA

10:50-11:05 A Fully Coupled Approach for Predicting Pollutants Formation Through Reactor Network Analysis

Alessandro Stagni, Alberto Cuoci, Alessio Frassoldati, Tiziano Faravelli, and Eliseo Ranzi, Politecnico di Milano, Italy

11:10-11:25 Transport Properties Effects on the Combustion of Lycopodium Particles

Milad Shokouhmand, Pantea Farokhzad, and Mehdi Bidabadi, Iran University of Science and Technology, Iran

Tuesday, April 9

Lunch Break

11:30 AM-1:00 PM

Attendees on their own

MS7

Detonation Dynamics and Structure - Part II of II

1:00 PM-3:00 PM

Room: Tango 2

For Part 1 see MS4

The accurate description of detonation evolution and structure in homogeneous and heterogeneous reactive media remains a significant challenge and a topic of ongoing research. Mathematical models typically involve nonlinear PDEs supplemented by non-ideal equations of state and stiff source terms. When reaction is strongly state-sensitive, instabilities are the norm and chemico-hydrodynamic coupling generates complex, unsteady structures. For heterogeneous explosives, or when the confining walls are compliant, accurate numerical treatment of multi-material and multi-phase models is an additional requirement. The talks will focus on adaptive, high-order numerical methods and well-resolved numerical results for a variety of problems including detonation initiation, stability, reflection, diffraction, response to confinement, and failure.

Organizer: Donald W. Schwendeman
Rensselaer Polytechnic Institute, USA

Organizer: Ashwani K. Kapila
Rensselaer Polytechnic Institute, USA

1:00-1:25 Adaptive High-resolution Simulation of Shock-induced Unsteady Hydrogen-air Combustion

Ralf Deiterding, Oak Ridge National Laboratory, USA; Bok Jik Lee, University of Cambridge, United Kingdom

1:30-1:55 Initiation of Viscous Detonation

Christopher Romick, University of Notre Dame, USA; Tariq Aslam, Los Alamos National Laboratory, USA; Joseph M. Powers, University of Notre Dame, USA

2:00-2:25 Modeling the Detonation Structure of Gaseous Detonations: What's Missing?

Matei I. Radulescu, University of Ottawa, Canada

2:30-2:55 Converging Detonation in a Radial Outflow

Aslan R. Kasimov and Svyatoslav Korneev, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

continued in next column

Tuesday, April 9

MS8

Hybrid CPU+Accelerator Simulation Techniques for Reacting Flows with Complex Chemical Kinetics

1:00 PM-3:00 PM

Room: Tango 1

Recent high performance computer systems have a heterogeneous architecture composed of multicore processors and GPUs as computational accelerators. The increase in computational power from the use of these modern architectures has the potential to improve the detail and fidelity of models used in simulating reacting flows. Efficiently harnessing the performance of hybrid architectures requires algorithmic and programming techniques that expose parallelism to the underlying hardware. In this minisymposium, we will discuss the experiences and results from developing software to utilize the GPUs for simulating reacting flows with complex chemical kinetics.

Organizer: Ramanan Sankaran
Oak Ridge National Laboratory, USA

1:00-1:25 Accelerated Computation of Detailed Chemical Reaction Kinetics for Complex Fuels

Ramanan Sankaran, Oak Ridge National Laboratory, USA; Ray W. Grout, National Renewable Energy Laboratory, USA

1:30-1:55 High Fidelity Simulations of Non-Equilibrium Plasma Flows with Complex Collisional-Radiative Kinetics

Jean-Luc Cambier, Air Force Research Laboratory, USA

2:00-2:25 Techniques for Solving Stiff Chemical Kinetics on GPUs

Christopher Stone, Computational Science and Engineering, LLC, USA

2:30-2:55 GPU Computing for Chemical Kinetics in Combustion CFD

Yu Shi, Phillips 66 Research Center, USA; Oluwayemisi Oluwale, ANSYS, Inc., USA; William H. Green, Massachusetts Institute of Technology, USA; Hsi-Wu Wong, Aerodyne Research, Inc., USA

Tuesday, April 9

CP14

Topological and Geometrical Modeling of Flames

1:00 PM-2:40 PM

Room: Tango 3

Chair: Luca Tosatto, Massachusetts Institute of Technology, USA

1:00-1:15 Topological Segmentation for Exploring Turbulence-Chemistry Interaction

Ray W. Grout, National Renewable Energy Laboratory, USA; P.-T. Bremer, Lawrence Livermore National Laboratory, USA; Gruber Andrea, SINTEF Energy Research, Norway; J.C. Bennett, Sandia National Laboratories, USA; A. Gyulassy, University of Utah, USA; H Kolla and J.H. Chen, Sandia National Laboratories, USA

1:20-1:35 Validation of a Fractal Dynamic Sgs Combustion Model for LES by DNS of Turbulent Jet and V-Shape Premixed Flames

Katsuhiro Hiraoka, Itaru Yoshikawa, Naoya Fukushima, Masayasu Shimura, Mamoru Tanahashi, and Toshio Miyauchi, Tokyo Institute of Technology, Japan

1:40-1:55 Simulation of Premixed Flames As Gasdynamic Discontinuities in Artificial Turbulent Flow Fields

Sabine Strein, Christian Bruzzese, and Andreas Class, Karlsruhe Institute of Technology, Germany

2:00-2:15 On the Fractal Properties of Low Damköhler Number Flames

Evatt R. Hawkes and Obulesu Chatakonda, University of New South Wales, Australia; Andrew Aspden, University of Portsmouth, United Kingdom; Alan Kerstein, Hemanth Kolla, and Jacqueline Chen, Sandia National Laboratories, USA

2:20-2:35 Scale-Space Analysis of Turbulent Flame Structures

Aaron P. Jackson, Alexei Poludnenko, and Elaine Oran, Naval Research Laboratory, USA

Tuesday, April 9

CP15

Detailed and Reduced Chemistry

1:00 PM-3:00 PM

Room: Tango 4

Chair: Shyam K. Menon, California Institute of Technology, USA

1:00-1:15 A Tabulated Chemistry Approach to Predict Transient Ignition Phenomena in Flammable Mixtures

Shyam K. Menon and Philipp Boettcher, California Institute of Technology, USA; Brian Ventura, Georgia Institute of Technology, USA; Guillaume Blanquart and Joseph E. Shepherd, California Institute of Technology, USA

1:20-1:35 Comparison of Reduced Chemistry and Tabulated Chemistry Modeling in Large-Eddy Simulation of a Two-Phase Experimental Burner

Benedetta G. Franzelli, Ecole Centrale Paris, France; Eleonore Riber and Bénédicte Cuenot, CERFACS, France; Benoit Fiorina and Nasser Darabiha, Ecole Centrale Paris, France

1:40-1:55 A Fast Method for Decoupled Species and Reaction Reduction in Adaptive Chemistry Combustion Simulations

Oluwayemisi Oluwale and Graham Goldin, ANSYS, Inc., USA

2:00-2:15 Fundamental Issues in Combustion Using Implicit Simulations with Realistic Chemistry: Flame-Pressure Interactions and Stretched Flame Speed

Nadeem Malik, King Fahd University of Petroleum and Minerals, Saudi Arabia

2:20-2:35 Detailed Numerical Study of the Effects of OH and O₂ Oxidation Rates on Soot Formation in Flames

Ali Khosousi, Ryerson University, Canada; Murray Thomson, University of Toronto, Canada; Seth Dworkin, Ryerson University, Canada

2:40-2:55 Identification of Critical Chemical Processes for Limit Flame Phenomena

Ruiqin Shan and Tianfeng Lu, University of Connecticut, USA

Tuesday, April 9

CP16

Direct Numerical Simulation

1:00 PM-3:00 PM

Room: Rumba

Chair: Jacqueline Chen, Sandia National Laboratories, USA

1:00-1:15 Investigation of Flame Kernel Expansion in a Stratified Mixture Using Dns

Catherine Gruselle, INSA Rouen, France;
Perrine Pepiot, Cornell University, USA;
Vincent Moureau and Yves D'Angelo, CORIA, France; Frédéric Ravet, Renault, France

1:20-1:35 On the Finite Differences Used in Combustion DNS

Robert Prosser, University of Manchester, United Kingdom

1:40-1:55 Dns of Turbulent Inhomogeneous-Reactant Premixed Flame with Complex Chemistry

Kian Min Lim and Stewart Cant, University of Cambridge, United Kingdom

2:00-2:15 Application of a PDF Method and DNS to Ignition Processes in Transient Turbulent Jets

Asghar Ghorbani, Physikalisch-Technische Bundesanstalt, Germany; Gordon Fru, University of Magdeburg, Germany; Detlef Markus, Physikalisch-Technische Bundesanstalt, Germany; Dominique Thévenin, University of Magdeburg, Germany; Ulrich Maas, Karlsruhe Institute of Technology, Germany

2:20-2:35 Large-Scale Modulation of Turbulent Bunsen Flames

Thiago Cardoso De Souza and Rob Bastiaans, Technische Universiteit Eindhoven, The Netherlands; Bernard Geurts, Twente University, Netherlands; Phillip de Goeij, Technische Universiteit Eindhoven, The Netherlands

2:40-2:55 DNS of Turbulent Oxy-fuel Flames -- Effects of Differential and Thermal Diffusion

Felix Dietzsch, Technische Universität Bergakademie Freiberg, Germany; Gordon Fru and Dominique Thevenin, Otto-von-Guericke-Universität Magdeburg, Germany; Christian Hasse, Technische Universität Bergakademie Freiberg, Germany

Sessions Conclude for Attendees to Explore San Antonio

3:00 PM

Wednesday, April 10

Registration

7:30 AM-4:00 PM

Room: Pre-function Area

Continental Breakfast

7:30 AM

Room: Skyline Atrium



Closing Remarks

8:10 AM-8:15 AM

Room: Tango 1 and 2

Wednesday, April 10

IP3

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

8:15 AM-9:00 AM

Room: Tango 1 and 2

Chair: Mitchell Smooke, Yale University, USA

This work 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 (speaker)

Alberto Cuoci

Alessio Frassoldati

Eliseo Ranzi

Politecnico di Milano, Italy

Coffee Break

9:00 AM-9:30 AM

Room: Skyline Atrium



Wednesday, April 10

MS9

Uncertainty Quantification in Numerical Combustion - Part III of IV

9:30 AM-11:30 AM

Room: Tango 1

For Part 2 see MS3

For Part 4 see MS12

Chemically reacting flow models involve a large number of parameters, which are typically estimated from experiments or computations. Quantifying uncertainties in these parameters, and associated computational predictions, is necessary for assessment of predictability in combustion models, for model selection and validation, and for enabling decision support. This minisymposium explores a wide range of topics in uncertainty quantification with particular focus on their application in computational reacting flow.

Organizer: Habib N. Najm
Sandia National Laboratories, USA

9:30-9:55 A Stochastic Flamelet Model for Reactive Flow Computations Under Uncertainty

Gianluca Iaccarino, Stanford University, USA

10:00-10:25 Applications of Global Sensitivity Analysis to Large Chemical-Kinetics Models and Beyond

Michael J. Davis, Argonne National Laboratory, USA

10:30-10:55 Inference-based Assessment of Ab Initio Rate Coefficient Calculations

Jens Prager, Habib N. Najm, Ewa Papajak, and Judit Zador, Sandia National Laboratories, USA

11:00-11:25 Uncertainty and Sensitivity Analysis for Turbulent Combustion of Hydrogen-rich Fuels

Kalen Braman, Todd Oliver, Venkat Raman, and Robert D. Moser, University of Texas at Austin, USA

Wednesday, April 10

CP17

Bio-Mass/Coal

9:30 AM-11:10 AM

Room: Tango 2

Chair: Philip Smith, University of Utah, USA

9:30-9:45 Computational Model of Biomass Co-Firing and Pollutant Development in a Pulverized Coal-Fired Boiler

Pavel Strachota, Michal Benes, and Tomas Oberhuber, Czech Technical University, Czech Republic; Vladimir Havlena, Honeywell Technology Center Europe, Czech Republic; Robert Straka, AGH University of Science and Technology, Poland

9:50-10:05 The Impact of Biomass Fuels on the Volatile Flame Length During Cofiring

Melissa Holtmeyer, Benjamin Kumfer, and Richard Axelbaum, Washington University in St. Louis, USA

10:10-10:25 CFD Modeling of Wood Sawdust Gasification in a Laboratory-Scale Fluidized Bed Reactor

Christos Altantzis, Addison Stark, and Ahmed F. Ghoniem, Massachusetts Institute of Technology, USA

10:30-10:45 Analysis of Ignition in Coal Combustion Process Using a One-Dimensional Turbulence Model

Babak Goshayeshi and James C. Sutherland, University of Utah, USA

10:50-11:05 Shock-Induced Combustion of Coal Dust Layers

Ryan Houim, National Research Council, USA; Elaine S. Oran, Naval Research Laboratory, USA

Wednesday, April 10

CP18

Compressible Reacting Flow

9:30 AM-10:50 AM

Room: Rumba

Chair: Joseph C. Oefelein, Sandia National Laboratories, USA

9:30-9:45 A Phenomenological Study of Detonation Phenomena in Porous Mixtures of Aluminum and Teflon

Sunhee Yoo, University of Illinois, USA; Scott Stewart and Sungjin Choi, University of Illinois at Urbana-Champaign, USA; Mario Fajardo, United States Air Force Academy, USA

9:50-10:05 Modeling Anisotropic Sensitivity in Pentaerythritol Tetranitrate Using Strain Rate Dependent Detonation Rate Law

Kihong Kim, Lawrence Livermore National Laboratory, USA, and Seoul National University, Korea; Laurence E. Fried, Lawrence Livermore National Laboratory, USA; Jack J. Yoh, Seoul National University, Korea

10:10-10:25 Numerical Study of Mixing and Combustion of Transverse Fuel Injection in Supersonic Mainstream

Yashar Shoraka and Sadegh Tabejamaat, Amirkabir University of Technology, Iran

10:30-10:45 Estimating Measurement Uncertainty in the Ignition Delay Time of Methane and Ethylene Mixtures Behind Reflected Shock Waves

David Sheen, University of Southern California, USA; Gaetano Esposito, University of Virginia, USA

Wednesday, April 10

CP19

Laminar Flames II

9:30 AM-11:10 AM

Room: Tango 3

Chair: Alberto Cuoci, Politecnico di Milano, Italy

9:30-9:45 Unsteady Effects in Laminar Premixed Flames with Transverse Mixture Stratification

Kian Min Lim, University of Cambridge, United Kingdom; Nilanjan Chakraborty, Newcastle University, United Kingdom; Stewart Cant, University of Cambridge, United Kingdom

9:50-10:05 Numerical Study of the Relation Between Chemiluminescence and Heat Release in Laminar Flames

Trupti Kathrotia and Uwe Riedel, German Aerospace Center, Stuttgart, Germany

10:10-10:25 Numerical Simulation of the Chemiluminescent Species in Lifted Tribrachial N-Heptane Laminar Flames with Heated Coflow

Fabrizio Bisetti, Mani Sarathy, Sukho Chung, Milan Toma, and Sungwoo Park, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

10:30-10:45 Calculation and Analysis of Electron Transport Properties Across Premixed Methane/air Flames

Mbark El Morsli, Jie Han, and Fabrizio Bisetti, King Abdullah University of Science & Technology (KAUST), Saudi Arabia

10:50-11:05 Numerical Studies of Methane-Air Mixture Ignition by Nanosecond Plasma Discharge

Maria Luis Castela, Benoit Fiorina, Olivier Gicquel, Christophe Laux, and Nasser Darabiha, Ecole Centrale Paris, France

Wednesday, April 10

CP20

Numerical Methods III

9:30 AM-11:30 AM

Room: Tango 4

Chair: Tariq Aslam, Los Alamos National Laboratory, USA

9:30-9:45 The Runge-Kutta-Legendre Method: Efficient Explicit Time Integration for Parabolic Partial Differential Equations

Tariq Aslam, Los Alamos National Laboratory, USA

9:50-10:05 Accelerating Stiff Chemical Kinetics in Combustion Simulations Using GPUs

Kyle E. Niemeyer, Case Western Reserve University, USA; Chih-Jen Sung, University of Connecticut, USA

10:10-10:25 A Time-Accurate Pressure Projection Method for Reacting Flows

Amir Biglari, Tony Saad, and James C. Sutherland, University of Utah, USA

10:30-10:45 On Spurious Numerics in Solving Reactive Equations

Dmitry Kotov, Stanford University, USA; Helen Yee, NASA Ames Research Center, USA; Wei Wang, Florida International University, USA; Chi-Wang Shu, Brown University, USA

10:50-11:05 Higher-Order Discontinuous Galerkin Method for Application to Realistic Combustion Problems

Yu Lv, University of Michigan, USA; Matthias Ihme, Stanford University, USA

11:10-11:25 Solving Degenerate Quenching-Combustion Equations Via Exponentially Evolving Grids (eeg)

Qin Sheng and Matthew Beauregard, Baylor University, USA

Lunch Break

11:30 AM-1:00 PM

Attendees on their own

Wednesday, April 10

MS10

Coal Combustion and Gasification: From Fundamental Processes to Technical Applications - Part II of II

1:00 PM-3:00 PM

Room: Tango 2

For Part 1 see MS6

Coal combustion and gasification are still the dominating processes to generate electrical base load power and chemical feedstocks. Further optimization of these high temperature conversion processes heavily relies on numerical modeling. CFD of thermal coal conversion requires reliable sub-models to account for turbulence, particle transport, pyrolysis, heterogeneous char reactions and homogeneous combustion. The first session focuses on recent sub-model developments. Also, needs for experimental benchmark data for model validation are presented. The second session focuses on CFD modeling. Target applications ranging from small laboratory flames to pilot scale furnaces are investigated looking at aspects such as coal flame structure and pollutant formation.

Organizer: Christian Hasse
Technische Universität Bergakademie Freiberg, Germany

Organizer: Oliver T. Stein
Universität Stuttgart, Germany

Organizer: Andreas Kempf
University of Duisburg-Essen, Germany

1:00-1:25 A Comparative Study of Large Eddy Simulations of a Pulverised Coal Jet Flame

Oliver T. Stein, Gregor Olenik, and Andreas Kronenburg, Universität Stuttgart, Germany; Marco Ghiani, Michele Vascellari, and Christian Hasse, Technische Universität Bergakademie Freiberg, Germany; Mario Franchetti and Fabrizio Cavallo Marincola, Imperial College London, United Kingdom; Andreas Kempf, University of Duisburg-Essen, Germany

continued on next page

1:30-1:55 Large-Eddy Simulation of a Pulverized Coal Combustion Field in a Furnace with a Realistic Strong Swirling Burner

Hiroaki Watanabe and Kenji Tanno, Central Research Institute of Electric Power Industry, Japan; Ryoichi Kurose, Kyoto University, Japan

2:00-2:25 From Descriptive to Predictive and Back Again: The Need for Both Fundamental and Empirical Models in Coal Gasification

Charles Reid, John Nitao, Julio Friedmann, and David Camp, Lawrence Livermore National Laboratory, USA; Philip Smith, University of Utah, USA

2:30-2:55 Virtual Dynamic Simulation of a Coal Fired Power Plant

M Pourkashanian, Leeds University, United Kingdom

Wednesday, April 10

CP21

Detonation I

1:00 PM-3:00 PM

Room: Tango 4

Chair: *Thomas Jackson*, University of Illinois at Urbana-Champaign, USA

1:00-1:15 Vibrational Relaxation Effects on Detonation Dynamics

Brian D. Taylor, David Kessler, Vadim N. Gamezo, and Elaine S. Oran, Naval Research Laboratory, USA

1:20-1:35 Detailed Simulation of Weak and Strong Ignition-Transition Behind a Bifurcating Shock-Wave

Matthias Ihme, Stanford University, USA; Yong Sun, University of Michigan, USA; Ralf Deiterding, Oak Ridge National Laboratory, USA

1:40-1:55 The Simulation of a Hydrogen-Bubble Reaction Due to Shock Ignition

Samuel Paolucci and Temistocle Grenga, University of Notre Dame, USA

2:00-2:15 Lead Shock Velocity and Curvature Variation in Weakly Unstable Detonation

Scott I. Jackson and Mark Short, Los Alamos National Laboratory, USA

2:20-2:35 A General Dead-Zone Predicted with the DSD Theory

Jin Yao, Lawrence Livermore National Laboratory, USA

2:40-2:55 Interaction of a Thin Detonation Wave with a Nonuniform Density Pattern

Cesar Huete, Universidad Carlos III de Madrid, Spain; Antonio L. Sanchez and Forman Williams, University of California, San Diego, USA

Wednesday, April 10

CP22

LES III

1:00 PM-3:00 PM

Room: Rumba

Chair: *Edward Knudsen*, Bosch Research And Technology Center, USA

1:00-1:15 Les Of A Premixed Jet Dns Using A Strained Flamelet Model

Edward Knudsen, Bosch Research And Technology Center, USA; Heinz Pitsch, RWTH Aachen University, Germany; Evatt R. Hawkes, University of New South Wales, Australia

1:20-1:35 LES Modeling of Stratified Flames Stabilized by Heat Losses

Renaud Mercier and Pierre Auzillon, Ecole Centrale Paris, France; Vincent Moureau, CORIA, France; Nasser Darabiha, Olivier Gicquel, Denis Veynante, and Benoit Fiorina, Ecole Centrale Paris, France

1:40-1:55 Assessment of Conditional Source-Term Estimation Method for Large-Eddy Simulation of Turbulent Premixed Flames

Nasim Shahbazian, University of Toronto, Canada; M. Mahdi Salehi, University of British Columbia, Canada; Clinton P. Groth, University of Toronto, Canada; W. Kendal Bushe, University of British Columbia, Canada

2:00-2:15 Large Eddy Simulation of a Supersonic Burner

Lisa Bouheraoua and Pascale Domingo, CORIA, France; Guillaume Ribert, INSA de Rouen, France

2:20-2:35 Large Eddy Simulation of Ignition in An Annular Multiple Injector Combustor

Thomas Schmitt, *Maxime Philip*, Matthieu Boileau, Ronan Vicquelin, Jean-Francois Bourgoin, Daniel Durox, and Sébastien Candel, Ecole Centrale Paris, France

2:40-2:55 LES of MILD Combustion: Delft Jet-in-Hot-Coflow Flame

Francisco E. Hernandez Perez, Jeroen van Oijen and Philip de Goey, Technische Universiteit Eindhoven, The Netherlands

Wednesday, April 10

CP23

Stability

1:00 PM-3:00 PM

Room: Tango 1

Chair: Viswanath Katta, Innovative Scientific Solutions, Inc., USA

1:00-1:15 Mathematical Investigation of Comustion Instability Due to Thermoacoustic Interaction in A Premixed Gas Turbine

Milad Shokouhmand and Pantea Farokhzad, Iran University of Science and Technology, Iran

1:20-1:35 Two-Dimensional Pulsating Instability of High Lewis Number Flames

Vadim N. Gamezo, Alexei Y. Poludnenko, and Elaine S. Oran, Naval Research Laboratory, USA; Forman Williams, University of California, San Diego, USA

1:40-1:55 Direct Numerical Simulation of the Instability of Explosively Expanding Material Interfaces

Fedir Sirotkin, Min-Cheol Gwak, and Jack J. Yoh, Seoul National University, Korea

2:00-2:15 Non-Linear and Linear Stability of Pulsating Overdriven Detonation with a Chain-Branching Kinetics Model

Carlos Chiquete and Mark Short, Los Alamos National Laboratory, USA

2:20-2:35 Response of a Transcritical Coaxial Flame Submitted to High-Frequency Transverse Acoustic Modulations

Thomas Schmitt and Loyal Hakim, Ecole Centrale Paris, France; Sebastien Ducruix, Laboratoire EM2C, France; Sébastien Candel, Ecole Centrale Paris, France

2:40-2:55 Analytical Methods for Solving the Problem of Thermal Explosion of Polydisperse Fuel Spray System in the Form of Singularly Perturbed System

Ophir Nave and Vladimir Goldshtein, Ben Gurion University Negev, Israel; Ajadi Suraju, Obafemi Awolowo University, Nigeria

Wednesday, April 10

CP24

Statistical and PDF Methods

1:00 PM-3:00 PM

Room: Tango 3

Chair: Rob Bastiaans, Technische Universiteit Eindhoven, The Netherlands

1:00-1:15 Comparison of Statistical Properties of Advected Diffusive Scalars and Advected Propagating Fronts, and Implications for Turbulent Premixed Flame Propagation

Alan Kerstein and Jackson Mayo, Sandia National Laboratories, USA

1:20-1:35 A Transport Equation for Flame Turbulence Interaction in Turbulent Premixed Flames

Umair Ahmed, Robert Prosser, and Alistair Revell, University of Manchester, United Kingdom

1:40-1:55 Statistical Behaviours of Scalar Dissipation Rate Transport Equation Terms for Turbulent Premixed Flames in the Context of Large Eddy Simulations

Nilanjan Chakraborty, Newcastle University, United Kingdom; Hemanth Kolla, Sandia National Laboratories, USA; Y Gao, Newcastle University, United Kingdom; Jacqueline Chen, Sandia National Laboratories, USA; N Swaminathan, University of Cambridge, United Kingdom

2:00-2:15 Transported Pdf Modeling for Oxy-Fuel Combustion

Xinyu Zhao and Daniel C. Haworth, Pennsylvania State University, USA

2:20-2:35 Evaluation of the Subgrid Pdf of the Progress Variable of Premixed Methane and Hydrogen Flames

Rob Bastiaans, Technische Universiteit Eindhoven, The Netherlands; Marc Day, Lawrence Berkeley National Laboratory, USA

2:40-2:55 Transported Probability Density Function Modeling for High-Efficiency Compression Ignition Engines

Vivek Raja Raj Mohan, Subhasish Bhattacharjee, and Daniel Haworth, Pennsylvania State University, USA

Coffee Break

3:00 PM-3:30 PM

Room: Skyline Atrium



Wednesday, April 10

MS11

Applications and Advances in One-dimensional Turbulence Simulation

3:30 PM-5:30 PM

Room: Tango 2

Turbulent combustion involves physical processes spanning device scales to dissipation scales where flames evolve. Flows with strong coupling between scales are notoriously difficult to model. The one-dimensional turbulence (ODT) model is unique in that a full range of scales are captured directly in physical space. ODT has been successfully applied to many flows and is under continuous development and extension. This minisymposium covers recent advances in ODT including comparisons to DNS; temperature statistics and fire spread in multiphase formulations; application to turbulent premixed flame speeds; and model extensions to three dimensional flows using coupled LES/ODT and ODT lattice approaches.

Organizer: David O. Lignell
Brigham Young University, USA

3:30-3:55 One-dimensional Turbulence Simulation: Advances and Application to Multi-phase Combustion

David O. Lignell, Brigham Young University, USA; John C. Hewson, Sandia National Laboratories, USA; Guangyuan Sun and Abinash Paudel, Brigham Young University, USA

4:00-4:25 The Contributions of LEM and ODT Toward a Better Understanding of Turbulent Flame Speeds

Heiko Schmidt, Brandenburgische Technische Universität Cottbus, Germany

4:30-4:55 One-Dimensional Turbulence: An Evaluation based on Comparisons with DNS Data for Turbulent Combustion

James C. Sutherland, University of Utah, USA

5:00-5:25 A ODT-Based Multiscale Framework for Turbulent Combustion Modeling

Tarek Echekki, North Carolina State University, USA

Wednesday, April 10

MS12

Uncertainty Quantification in Numerical Combustion - Part IV of IV

3:30 PM-5:30 PM

Room: Tango 1

For Part 3 see MS9

Chemically reacting flow models involve a large number of parameters, which are typically estimated from experiments or computations. Quantifying uncertainties in these parameters, and associated computational predictions, is necessary for assessment of predictability in combustion models, for model selection and validation, and for enabling decision support. This minisymposium explores a wide range of topics in uncertainty quantification with particular focus on their application in computational reacting flow.

Organizer: Habib N. Najm
Sandia National Laboratories, USA

3:30-3:55 Estimating and Utilizing Uncertainties in Theoretically Predicted Rate Coefficients

Stephen Klippenstein, C. Franklin Goldsmith, and Michael P. Burke, Argonne National Laboratory, USA; Alison S. Tomlin, Leeds University, United Kingdom; Lawrence B. Harding, Argonne National Laboratory, USA

4:00-4:25 Deterministic Uncertainty Quantification Using Rational-quadratic Surrogate Models: Response Surface Modeling and Inference

Andrew Packard, University of California, Berkeley, USA

4:30-4:55 Comparative Analysis of Uncertainties Associated with Transport and Chemical Kinetics in Laminar Flames

Gaetano Esposito and Harsha Chelliah, University of Virginia, USA

5:00-5:25 Parameter Estimation with Missing Data

Habib N. Najm, Cosmin Safta, Khachik Sargsyan, Bert J. Debusschere, and Kenny Chowdhary, Sandia National Laboratories, USA

Wednesday, April 10

CP25

Detonation II

3:30 PM-5:10 PM

Room: Tango 4

Chair: Brandon A. Lieberthal, University of Illinois at Urbana-Champaign, USA

3:30-3:45 Modeling Detonation of Heterogeneous Explosives with Embedded Inert Particles Using Detonation Shock Dynamics

Brandon A. Lieberthal, Scott Stewart, and John Bdzil, University of Illinois at Urbana-Champaign, USA

3:50-4:05 Development of Detonation Rate Model for Selective Energetic Materials Subject to External Impact

Bohoon Kim and Jack J. Yoh, Seoul National University, Korea

4:10-4:25 Spontaneous Deflagration-to-Detonation Transition in Thermonuclear Supernovae

Alexei Poludnenko, Vadim N. Gamezo, and Elaine S. Oran, Naval Research Laboratory, USA

4:30-4:45 Pore Collapse in Explosive Materials and the Generation of Detonations

John D. Buckmaster, Buckmaster Research, USA; Thomas Jackson, University of Illinois at Urbana-Champaign, USA

4:50-5:05 Modeling and Numerical Simulations for Product Species Identification in Mezo-Scale Reactions of Energetic Materials

Sungjin Choi, Sunhee Yoo, D. Scott Stewart, and Nick G. Glumac, University of Illinois at Urbana-Champaign, USA

Wednesday, April 10

CP26

Flamelets II

3:30 PM-4:50 PM

Room: Rumba

Chair: Hemanth Kolla, Sandia National Laboratories, USA

3:30-3:45 Spatially Filtered Flamelets Applied to Premixed Turbulent Combustion

Sudipto Mukhopadhyay, Rob Bastiaans, Jeroen Oijen, and Philip de Goey, Technische Universiteit Eindhoven, The Netherlands

3:50-4:05 Numerical Simulation of Turbulent Hydrogen Combustion Based on Flamelet Generated Manifolds with Open Foam

Alessio Fancello, R.J.M. Bastiaans, and L.P.H. De Goey, Eindhoven University of Technology, Netherlands

4:10-4:25 A Priori Assessment of Empirical Manifolds for Flamelet Modelling of Turbulent Premixed Combustion

Hemanth Kolla, Sandia National Laboratories, USA; Edward Knudsen, Bosch Research And Technology Center, USA; Jacqueline Chen, Sandia National Laboratories, USA

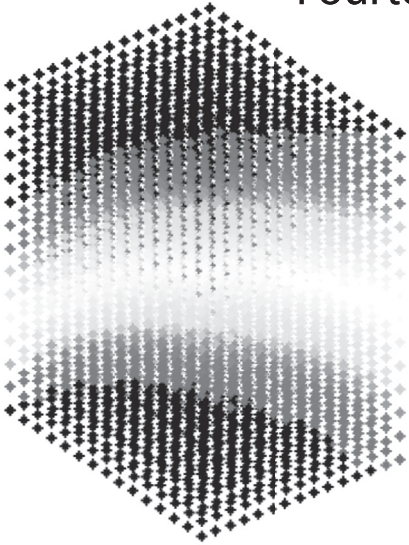
4:30-4:45 Predicting Sooting Tendencies with a New Flamelet-Based Model

Yuan Xuan and Guillaume Blanquart, California Institute of Technology, USA

Notes

NC13 Abstracts

Fourteenth International Conference on



NUMERICAL COMBUSTION

April 8-10, 2013

Holiday Inn San Antonio - Riverwalk
San Antonio, Texas, USA

Figure courtesy J. Breidt, T. Butler and D. Estep, SINUM Vol. 49, No. 5

Abstracts are printed as submitted by the author.

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

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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

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IP3**Numerical Modeling of Pollutant Emissions with Detailed Kinetics: from Ideal Reactors to Flames**

This work 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

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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.

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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

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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

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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.

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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.

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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.

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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 often 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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%.

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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.

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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.

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CP4

Extinction and Reignition in Turbulent Non-premixed 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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 level-set/progress variable model (Knudsen et al.). The focus is the evaluation of different models for the turbulent burning velocity.

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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.

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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.

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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.

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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.

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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.

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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.

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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 contribu-

tions 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*.

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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, NO_x, 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.

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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.

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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 combustor 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.

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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.

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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 is 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 δ . 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 δ . 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 negative 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 .

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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.

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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.

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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.

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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.

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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.

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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 instantaneous and must partially resolve the turbulent spectrum according to the available grid resolution and the chosen time step. This is usually 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.

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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.

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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.

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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.

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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.

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CP12

Interface Tracking of a Chemical Reacting Carbon Particle Moving in CO₂ 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 CO₂ and N₂. 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.

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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.

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CP12

Implementation of Unsteady Plug Flow Reactors in Cantera

In Cantera the reactor object is zero-dimensional, hence implementation of 1-dimensional plug flow 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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 Zel'dovich 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.

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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.

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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.

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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 theoretical and experimental results relating to flames at higher Damköhler number. The results are explained by theoretical arguments from two different viewpoints.

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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.

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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.

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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.

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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.

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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.

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CP15

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

Fundamental issues in combustion may be investigated 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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-Dimensional Turbulence (ODT) model. Detailed particle models for vaporization, devolatilization and char oxidation/gasification 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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 rapid mixing, and, consequently enhances the flame stabilization. Therefore, mixing and combustion of transverse fuel injection in supersonic mainstream is numerically investigated in the current research.

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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.

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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.

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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.

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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.

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CP19**Numerical Study of the Relation Between Chemi-****luminescence 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.

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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.

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CP20**The Runge-Kutta-Legendre Method: Efficient Explicit Time Integration for Parabolic Partial Differential Equations**

Stabilized Runge-Kutta time integration methods (also known 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.

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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.

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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 N_s-1 number of species variables (N_s 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.

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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 accurately 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.

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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.

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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.

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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.

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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.

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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.

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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.

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CP21

Vibrational Relaxation Effects on Detonation Dynamics

Recent time-dependent, multidimensional simulations of detonations in H₂-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.

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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.

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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.

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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.

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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.

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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).

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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CP24

A Transport Equation for Flame Turbulence Interaction in Turbulent Premixed Flames

In premixed turbulent combustion scalar dissipation $\tilde{\epsilon}_c$ 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 $\tilde{\epsilon}_c$ in premixed turbulent combustion.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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

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

Here the sensitivity parameters a, b for density and pressure, respectively are specified theoretically by the physico-chemical 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.

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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.

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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.

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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.

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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.

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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.

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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.

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MS1

Reaction Pathway Analysis Using Stochastic Sampling

Abstract not available at time of publication.

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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.

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MS1

Determination of the Uncertainty of Reaction Rate Parameters

Abstract not available at time of publication.

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MS1

Uncertainty Quantification Applied to Combustion Experiment Design

Abstract not available at time of publication.

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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.

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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 NO_x 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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MS4

Some Advances on Numerical Methods for Hyperbolic Balance Laws and Applications

Abstract not available at time of publication.

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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.

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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.

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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.

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MS5

Possibility of Kinetics Study in Tubes

As a spin-off technology from microcombustion, a micro-flow 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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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.

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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 thereby add an additional level of parallelism available for better utilization of the modern multicore and many core processors.

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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.

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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.

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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.

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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 work performed in collaboration with many researchers, particularly: Dingyu Zhou, Rex Skodje, Wei Liu, Raghu Sivaramakrishnan, Sibendu Som, and Douglas Longman.

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MS9

A Stochastic Flamelet Model for Reactive Flow Computations Under Uncertainty

Abstract not available at time of publication.

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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.

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MS10

Virtual Dynamic Simulation of a Coal Fired Power Plant

Today's 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.

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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.

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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

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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, NO_x 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.

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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.

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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.

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MS11

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

Abstract not available at time of publication.

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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.

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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.

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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.

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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 bars 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.

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MS12

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

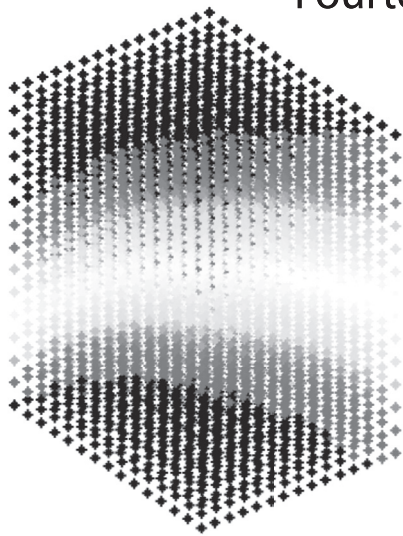
Abstract not available at time of publication.

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Notes

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Figure courtesy J. Breidt, T. Butler and D. Estep, SINUM Vol. 49, No. 5



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 Echekki, Tarek, MS11, 5:00 Wed
 Eguz, Ulas, CP2, 10:10 Mon
 El Morsli, Mbark, CP19, 10:30 Wed

F

Fancello, Alessio, CP26, 3:50 Wed
 Faravelli, Tiziano, IP3, 8:15 Wed
 Fernandez-Tarrazo, Eduardo, CP2, 10:50 Mon
 Fiorina, Benoit, CP7, 1:20 Mon
 Fischer, Marileen L., CP1, 9:30 Mon
 Fletcher, Tom, MS6, 10:00 Tue
 Franzelli, Benedetta G., CP15, 1:20 Tue

G

Gaillard, Pierre, CP5, 1:40 Mon
 Galagali, Nikhil, MS3, 5:00 Mon
 Gamezo, Vadim N., CP23, 1:20 Wed
 Ghorbani, Asghar, CP16, 2:00 Tue
 Gonzalez, Esteban, CP4, 9:50 Mon
 Goshayeshi, Babak, CP17, 10:30 Wed
 Goussis, Dimitris, IP2, 8:15 Tue
 Groth, Clinton P., CP3, 10:10 Mon
 Grout, Ray W., CP14, 1:00 Tue
 Gruselle, Catherine, CP16, 1:00 Tue

H

Hakim, Layal, CP23, 2:20 Wed
 Hasse, Christian, MS6, 9:30 Tue

Hasse, Christian, MS10, 1:00 Wed

Hawkes, Evatt R., CP14, 2:00 Tue
 Haworth, Daniel C., CP13, 9:30 Tue
 Hendra, Graham R., CP7, 2:40 Mon
 Hernandez Perez, Francisco E., CP22, 2:40 Wed
 Heye, Colin, CP11, 9:50 Tue
 Hiraoka, Katsuhiko, CP14, 1:20 Tue
 Holtmeyer, Melissa, CP17, 9:50 Wed
 Hossein Zadeh, Arash, CP9, 4:50 Mon
 Houim, Ryan, CP17, 10:50 Wed
 Huete, Cesar, CP21, 2:40 Wed
 Hunger, Franziska, CP5, 1:00 Mon

I

Iaccarino, Gianluca, MS9, 9:30 Wed
 Ihme, Matthias, CP21, 1:20 Wed

J

Jackson, Aaron P., CP14, 2:20 Tue
 Jackson, Scott I., CP21, 2:00 Wed
 Jackson, Thomas, CP25, 4:30 Wed
 Jalaal, Maziyyar, CP8, 3:50 Mon
 Jay, Stephane, CP2, 9:50 Mon
 Johnstone, Elizabeth R., MS4, 5:00 Mon

K

Kapila, Ashwani K., MS4, 3:30 Mon
 Kapila, Ashwani K., MS7, 1:00 Tue
 Kasimov, Aslan R., MS7, 2:30 Tue
 Kathrotia, Trupti, CP19, 9:50 Wed
 Katta, Viswanath R., CP5, 1:20 Mon
 Kempf, Andreas, MS10, 1:00 Wed
 Kempf, Andres, MS6, 9:30 Tue
 Kerstein, Alan, CP24, 1:00 Wed
 Ketelheun, Anja, CP7, 2:00 Mon
 Khosousi, Ali, CP15, 2:20 Tue
 Kim, Bohoon, CP25, 3:50 Wed
 Kim, Kihong, CP18, 9:50 Wed
 Klippenstein, Stephen, MS12, 3:30 Wed
 Knudsen, Edward, CP22, 1:00 Wed
 Kolla, Hemanth, CP24, 1:40 Wed
 Kolla, Hemanth, CP26, 4:10 Wed

Kotov, Dmitry, CP20, 10:30 Wed
 Koundinyan, SushilKumar P., CP5, 2:20 Mon
 Kurdyumov, Vadim, MS5, 10:30 Tue

L
 Labahn, Jeffrey, CP6, 1:40 Mon
 Lamouroux, Jean, MS2, 2:30 Mon
 Lieberthal, Brandon A., CP25, 3:30 Wed
Lignell, David O., MS11, 3:30 Wed
 Lignell, David O., MS11, 3:30 Wed
 Lim, Kian Min, CP16, 1:40 Tue
 Lim, Kian Min, CP19, 9:30 Wed
 Lv, Yu, CP20, 10:50 Wed
 Lyra, Sgouria, CP4, 10:30 Mon

M
 Ma, Dominic, CP6, 1:20 Mon
 Malik, Nadeem, CP15, 2:00 Tue
 Maragkos, Georgios, CP5, 2:00 Mon
 Martínez-Ruiz, Daniel, CP8, 4:30 Mon
Maruta, Kaoru, MS5, 9:30 Tue
 Maruta, Kaoru, MS5, 11:00 Tue
 Menon, Shyam K., CP15, 1:00 Tue
 Mercier, Renaud, CP22, 1:20 Wed
 Messig, Danny, CP9, 4:10 Mon
 Messig, Danny, CP9, 5:10 Mon
 Michael, Louisa, MS4, 4:30 Mon
 Mikolaitis, David W., CP12, 9:50 Tue
 Mitsingas, Constandinos M., CP1, 10:10 Mon
 Mogo, César, CP2, 11:10 Mon
 Mueller, Michael E., CP13, 10:30 Tue
 Mukhopadhyay, Sudipto, CP26, 3:30 Wed

N
Najm, Habib N., MS1, 1:00 Mon
Najm, Habib N., MS3, 3:30 Mon
Najm, Habib N., MS9, 9:30 Wed
Najm, Habib N., MS12, 3:30 Wed
 Najm, Habib N., MS12, 5:00 Wed
 Navarro-Martinez, Salvador, CP4, 9:30 Mon

Nave, Ophir, CP23, 2:40 Wed
 Niemeyer, Kyle E., CP20, 9:50 Wed
 Nivarti, Girish V., CP7, 1:40 Mon
O
 Oefelein, Joseph C., CP8, 3:30 Mon
 Oluwole, Oluwayemisi, CP15, 1:40 Tue
 Oster, Timo, CP12, 9:30 Tue

P
 Packard, Andrew, MS12, 4:00 Wed
 Paolucci, Samuel, CP21, 1:40 Wed
Parente, Alessandro, MS2, 1:00 Mon
 Parente, Alessandro, MS2, 1:00 Mon
 Philip, Maxime, CP22, 2:20 Wed
 Poludnenko, Alexei, CP25, 4:10 Wed
 Pourkashanian, M, MS10, 2:30 Wed
 Prosser, Robert, CP16, 1:20 Tue

R
 Radulescu, Matei I., MS7, 2:00 Tue
 Raj Mohan, Vivek Raja, CP24, 2:40 Wed
 Regele, Jonathan D., CP2, 10:30 Mon
 Reid, Charles, MS10, 2:00 Wed
 Ribert, Guillaume, CP11, 9:30 Tue
 Rizzi, Francesco, MS3, 4:00 Mon
 Rochoux, Melanie C., CP11, 10:30 Tue
 Romick, Christopher, MS7, 1:30 Tue
 Roy, Somesh P., CP13, 10:10 Tue

S
 Saghaffian, Amirreza, CP6, 1:00 Mon
Sankaran, Ramanan, MS8, 1:00 Tue
 Sankaran, Ramanan, MS8, 1:00 Tue
 Schmidt, Heiko, MS11, 4:00 Wed
 Schoch, Stefan, MS4, 5:30 Mon
Schwendeman, Donald W., MS4, 3:30 Mon
 Schwendeman, Donald W., MS4, 3:30 Mon
Schwendeman, Donald W., MS7, 1:00 Tue
 See, Yee Chee, CP11, 10:10 Tue
 Shaddix, Christopher, MS6, 11:00 Tue

Shahbazian, Nasim, CP22, 1:40 Wed
 Shan, Ruiqin, CP15, 2:40 Tue
 Sheen, David, CP18, 10:30 Wed
 Sheng, Qin, CP20, 11:10 Wed
 Shi, Yu, MS8, 2:30 Tue
 Shokouhmand, Milad, CP13, 11:10 Tue
 Shokouhmand, Milad, CP23, 1:00 Wed
 Shoraka, Yashar, CP18, 10:10 Wed
 Sirotkin, Fedir, CP23, 1:40 Wed
 Skodje, Rex, MS1, 1:30 Mon
 Smith, Philip J., MS3, 4:30 Mon
 Speth, Raymond L., CP12, 10:30 Tue
 Stagni, Alessandro, CP13, 10:50 Tue
 Stark, Addison, CP17, 10:10 Wed
Stein, Oliver T., MS6, 9:30 Tue
Stein, Oliver T., MS10, 1:00 Wed
 Stein, Oliver T., MS10, 1:00 Wed
 Stone, Christopher, MS8, 2:00 Tue
 Strachota, Pavel, CP17, 9:30 Wed
 Strein, Sabine, CP14, 1:40 Tue
Sutherland, James C., MS2, 1:00 Mon
 Sutherland, James C., MS11, 4:30 Wed

T
 Taylor, Brian D., CP21, 1:00 Wed
 Toro, Eleuterio F., MS4, 4:00 Mon
 Tosatto, Luca, MS1, 1:00 Mon
 Trisjono, Philipp, CP7, 1:00 Mon
 Turanyi, Tamas, MS1, 2:30 Mon

V
 Valiev, Damir M., CP4, 11:10 Mon
 Valorani, Mauro, MS3, 3:30 Mon
 Van Essendelft, Dirk, MS6, 10:30 Tue
 Vascellari, Michele, MS6, 9:30 Tue
 Vogiatzaki, Konstantina, CP6, 2:00 Mon

W
 Wang, Hai, MS1, 2:00 Mon
 Wasserman, Mark, CP3, 10:30 Mon
 Watanabe, Hiroaki, MS10, 1:30 Wed

X

Xuan, Yuan, CP9, 3:50 Mon

Xuan, Yuan, CP26, 4:30 Wed

Y

Yang, Yue, MS2, 2:00 Mon

Yao, Jin, CP21, 2:20 Wed

Yee, Helen, CP12, 10:50 Tue

Yoo, Sunhee, CP18, 9:30 Wed

Z

Zador, Judit, MS9, 10:30 Wed

Zhao, Xinyu, CP24, 2:00 Wed

NC13 Budget

Conference Budget SIAM Conference on Numerical Combustion April 8 - 10, 2013 San Antonio, TX

Expected Paid Attendance: 150

Revenue

Registration Income		\$60,885	
	Total	\$60,885	

Expenses

Printing	\$1,000	
Organizing Committee	\$1,900	
Invited Speakers	\$4,100	
Food and Beverage	\$24,000	
AV Equipment and Telecommunication	\$13,500	
Advertising	\$3,500	
Conference Labor (including benefits)	\$24,880	
Other (supplies, staff travel, freight, misc.)	\$2,900	
Administrative	\$8,649	
Accounting/Distribution & Shipping	\$6,069	
Information Systems	\$8,267	
Customer Service	\$3,113	
Marketing	\$5,060	
Office Space (Building)	\$3,395	
Other SIAM Services	\$3,787	
	Total	\$114,120

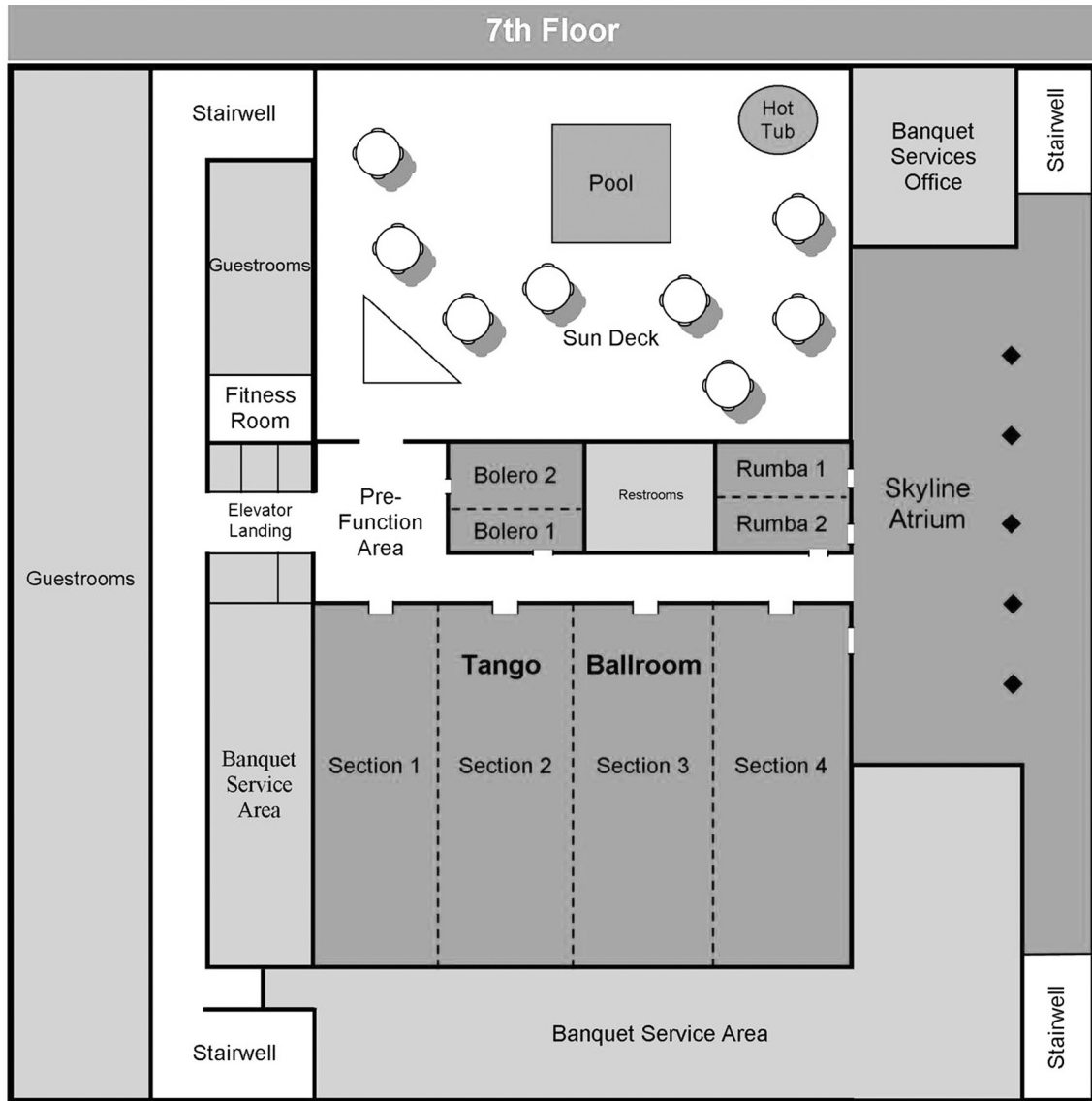
Net Conference Expense		-\$53,235	
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Support Provided by SIAM		\$53,235	
		\$0	

Estimated Support for Travel Awards not included above:

Post Docs and Students	7	\$5,000	
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Holiday Inn San Antonio-Riverwalk Floor Plan



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