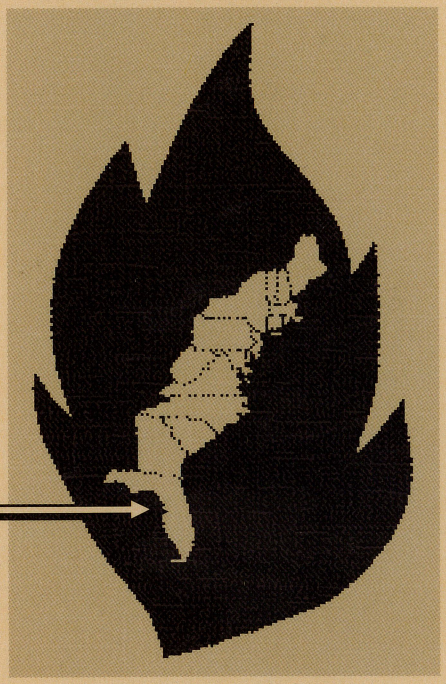
Chemical and Physical Processes of Combustion

The 2005 Technical Meeting of the Eastern States Section of the Combustion Institute

University of Central Florida



Orlando, Florida
November 13-15, 2005

Eastern States Section Officers, 2003-2005

Chair:	Mitchell Smooke, Yale University
Vice Chair:	Nicholas P. Cernansky, Drexel University
Secretary:	W. Terry Rawlins, Physical Sciences, Inc.
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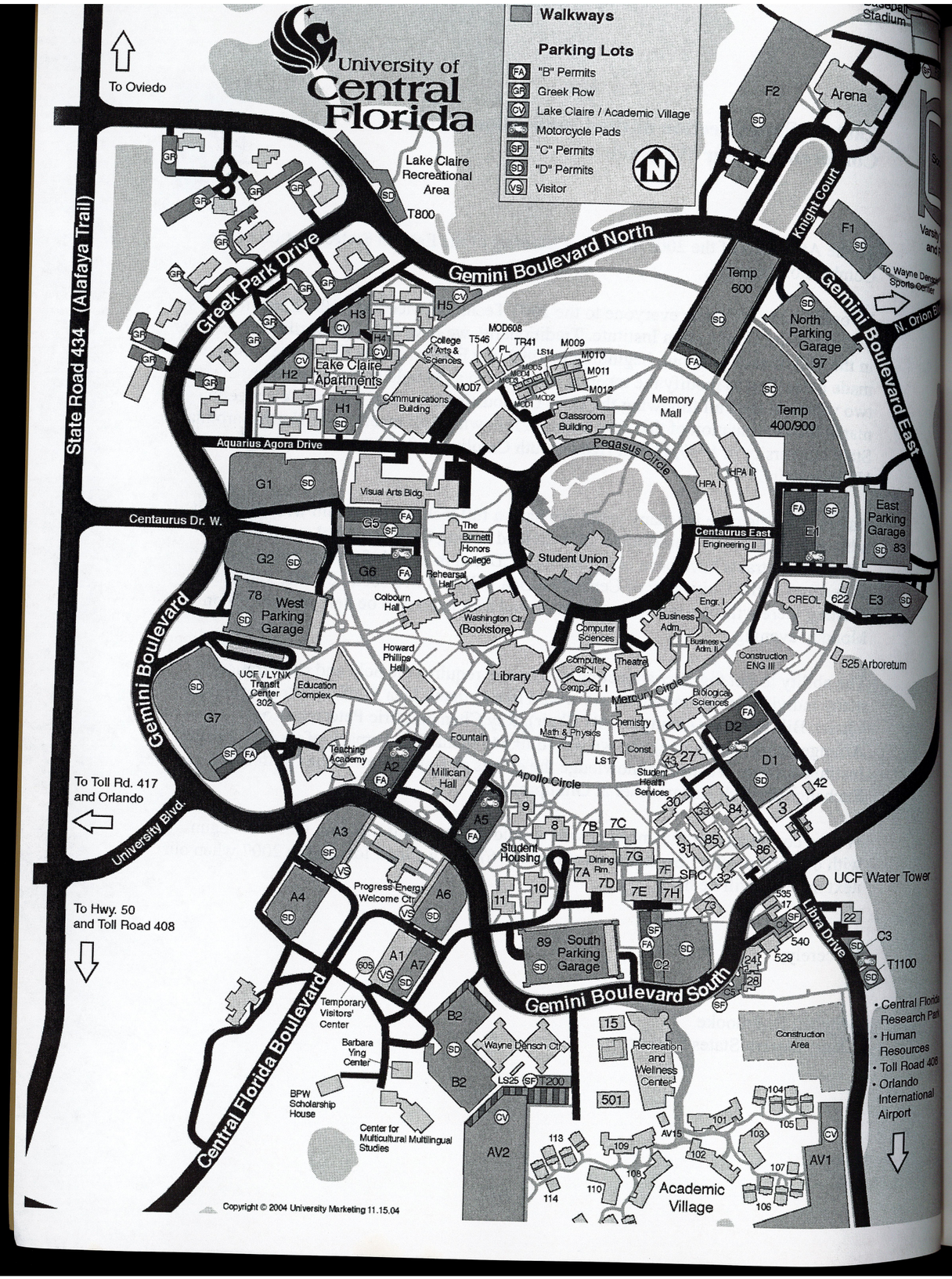
Program/Papers Chair:	Lisa Pfefferle, Yale University
Arrangements Chair:	Bill Roberts, North Carolina State University



Program Summary

Sunday, 13 November 2005

6:00-9:00 PM **Registration and welcome reception.**

Monday, 14 November 2005
Invited Talk 1 **Cape Florida Room (#316)**

8:30 AM *Welcoming Remarks*
8:45 AM *Combustion Chemistry Models and Data: A New Paradigm for the 21st Century* 1
William H. Green, MIT

Chemical Kinetics (Key West Room, 218A)
Chair: Eric L. Petersen, University of Central Florida

9:45 AM *Theoretical Study of the Kinetics and Mechanism for the Radical Reaction of $C_2H_5O_1$ with H* 2
Kun Xu, Zhen Feng Xu, M. C. Lin, Department of Chemistry, Emory University

10:05 AM *Ab Initio Kinetics for the Unimolecular Reaction $C_6H_5OH \rightarrow CO + C_5H_6$* 3
Zhen Feng Xu, M. C. Lin, Department of Chemistry, Emory University

10:25 AM *1,5-Hexadiyne and Fulvene Presence in Premixed Allene and Propyne Flames* 4
Matthew E. Law, Saugata Gon, Phillip R. Westmoreland, University of Massachusetts Amherst, Terrill A. Cool, Juan Wang Cornell University, Nils Hansen, Sandia National Laboratories

10:45 AM **Break.**

11:05 AM *Theoretical Study on the Reaction of CH_3OH with OH Radical* 8
Shucheng Xu, M.C. Lin, Emory University

11:25 AM *Theoretical Study Of Hydrogen Abstraction From Dimethyl Ether By OH Radical: Precious Rate Constant Predictions* 9
Shucheng Xu, M.C. Lin, Emory University

11:45 AM *Kinetics of the Thermal Decomposition of t-Butyl-1,3-Cyclopentadiene: Ring Expansion and Radical Formation* 10
W. Sean McGivern, Jeffrey A. Manion, Wing Tsang, National Institute of Standards and Technology

Turbulence and Fire Topics: Special Talk on World Trade Center (Key West Room, 218B)
Chair: William L. Roberts, North Carolina State University

9:45 AM *Micro-Vortex/Flame Interactions and Their Implications in Turbulent-Flame Modeling* 14
Viswanath R. Katta, Terrence Meyer, Innovative Scientific Solutions, Inc
William Roquemore, Air Force Research Laboratory

10:05 AM *A Comparison of Turbulent Premixed Combustion Models* 18
Scott M. Martin, Siemens Power Corporation

10:25 AM *Ignition of Vegetation and Mulch by Firebrands in Wildland/Urban Interface (WUI) Fires* 22
Samuel L. Manzello, Thomas Cleary, John Shields, Jiann C. Yang, National Institute of Standards and Technology

10:45 AM **Break.**

11:05 AM *Use of Visual Imagery for the NIST World Trade Center Investigation* 23

William M. Pitts, Kathryn M. Butler, Valentine Junker, National Institute of Standards and Technology

Ignition/Extinction (Key West Room, 218C)
Chair: David L. Miller, Drexel University

9:45 AM *Ignition Delay of Oxygenated Fuel Droplets*
Matthew Hammill, Timothy Vaughn, Anthony Marchese, Rowan University

10:05 AM *A Shock-Tube Study of The Ignition and Oxidation Characteristics of Syngas at Elevated Pressures*
Danielle M. Kalitan, Eric L. Petersen, University of Central Florida, John D. Mertens, Trinity College

10:25 AM *Effect of Higher-Order Hydrocarbons on the Ignition of Lean Methane-Air Mixtures at Elevated Pressures*
Eric L. Petersen, Danielle Kalitan, Stefanie Simmons, University of Central Florida , Henry J. Curran, National University of Ireland

10:45 AM **Break.**

11:05 AM *Lewis Number Effects on the Extinction of Counterflow Diffusion Flames*
Marcos Chaos, Princeton University, Ruey-Hung Chen, University of Central Florida

11:25 AM *Laser Ignition of Hydrogen Diffusion Jet Flame Diluted with Nitrogen*
Phuoc X. Tran, Fredrick, P White, DOE/NETL

11:45 AM *Computational Singular Perturbation Analysis of n-Heptane Two-Stage Ignition*
Andrei Kazakov, Marcos Chaos, Zhenwei Zhao, Frederick L. Dryer, Princeton University

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Invited Talk 2 **Cape Florida Room (#316)**

1:30 PM *Flame Synthesis of Nanostructured Materials*
Stephen Tse, Rutgers University

Soot (Key West Room, 218A)
Chair: Baki Cetegen, University of Connecticut

2:30 PM *Effects of Pressure on Mechanisms of Soot Surface Growth and Oxidation in Laminar Non-Premixed Flames at 1.0-8.0 atm*
C.H. Kim, G.M. Faeth, University of Michigan , F. Xu, University of Central Florida

2:50 PM *The Effects of Dimethyl Ether and Ethanol on Benzene and Soot Formation in Ethylene Nonpremixed Flames*
Charles S. McEnally, Lisa D. Pfefferle, Yale University

3:10 PM *Soot Reduction by NO_2 in a Laminar Premixed Flame*
Arvind V. Menon, Milton J. Linevsky, Matthew McKeand, Suresh S. Iyer, Seong-Young Lee, Thomas A. Litzinger, Robert J. Santoro, Pennsylvania State University

3:30 PM **Break.**

3:50 PM *Soot Distributions in a Planar Diffusion Flame Wrapped by a Line Vortex*
Saptarshi Basu, Baki M. Cetegen, University of Connecticut

4:10 PM *Transient Dynamics of Soot in Ethylene-Air Nonpremixed Counterflow Flames*
Chun Sang Yoo, Hong G. Im, University of Michigan

4:30 PM *Are the Fractal Characteristics of Soot Constant?*
Suresh S. Iyer, Thomas A Litzinger, Robert J Santoro, Pennsylvania State University

4:50 PM *Measurement of Smoke Point in Velocity-Matched Co-Flow Laminar Diffusion Flames with Pure and Diluted Fuels at Elevated Pressures*
T.L. Berry, W. L. Roberts, North Carolina State University

5:30-6:00 PM **Business meeting (Key West Room, 218A).**
7:30 PM **Banquet (Cape Florida Room, 316).**

Mechanisms and Reduced Mechanisms (Key West, Room 218B)
Chair: W. Sean McGivern, NIST

2:30 PM *Reduced High-Temperature Mechanisms for Large Paraffins – n-Hexadecane* 82
Marcos Chaos, Andrei Kazakov, Zhenwei Zhao, Frederick L. Dryer, Princeton University, Stephen P. Zeppieri, Technologies Research Center

2:50 PM *Application Of The ICE-PIC Method For The Dimension Reduction Of Chemical Kinetics* 86
Zhuyin Ren, Stephen B. Pope, Cornell University

3:10 PM *Obtaining Accurate Solutions Using Reduced Chemical Kinetic Models* 90
William H. Green, O.O. Oluwole, MIT

3:30 PM **Break.**

3:50 PM *Development of a Chemical Kinetics Mechanism for CH_4/H_2/Air Ignition at Elevated Pressures* 92
Joel M. Hall, Eric L. Petersen, University of Central Florida

4:10 PM *Insights Into a Premixed Stoichiometric Cyclohexane Flame* 96
Matthew E. Law, Phillip R. Westmoreland, University of Massachusetts Amherst, Terrill A. Cool, Juan Wang, Cornell University, Nils Hansen, Craig A. Taatjes, National Laboratories, Tina Kasper, Universität Bielefeld

4:30 PM *An Investigation of the Suppression Mechanism of CF_3Br Using the Reduced Kinetic Mechanisms for Premixed Hydrogen-Air-CF_3Br Flames* 100
Fang Xu, Yi Zhang, Zhiliang Li, University of Central Florida

4:50 PM *An Existing Global Heptane Mechanism Augmented with Diffusive Transport* 104
Howard Pearlman, Michael Foster, Drexel University

5:30-6:00 PM **Business meeting (Key West Room, 218A).**
7:30 PM **Banquet (Cape Florida Room, 316).**

Propellants and Detonations (Key West Room, 218C)
Chair: Thomas A. Litzinger, The Pennsylvania State University

2:30 PM *Confined Rapid Thermolysis/FTIR/ToF Studies of Imidazolium-based Ionic Liquids* 108
Arindrajit Chowdhury, Stefan T. Thynell, Pennsylvania State University

2:50 PM *Confined Rapid Thermolysis/FTIR/ToF Studies of Triazolium-based Ionic Liquids* 112
Arindrajit Chowdhury, Stefan T. Thynell, Pennsylvania State University

3:10 PM *Laser-driven Decomposition and Combustion of 4-Amino-1,2,4-Triazolium Nitrate* 116
Jianquan Li, Thomas A. Litzinger, Pennsylvania State University

3:30 PM **Break.**

3:50 PM *Impact of Nanoscale Aluminum on the Burn Rate of Composite Propellants Manufactured using Conventional Mixing Techniques* 120
Alexander R. P. LePage, M. Stephens, University of Central Florida

4:10 PM *Kinetics for the Combustion Initiation Reaction of Ammonium Perchlorate in the Condensed Phase* 124
R. S. Zhu, M. C. Lin, Emory University

4:30 PM *Curvature Effects On Detonations With Mole Decrement Reactions* 125
Viktor Gorchkov, Mark Short, University of Illinois at Urbana-Champaign

4:50 PM *Linear Stability Analysis of ZND Detonation Waves in General Reactive Systems* 129
Charles B. Kiyanda, Mark. Short, University of Illinois at Urbana-Champaign

5:30-6:00 PM **Business meeting (Key West Room, 218A).**
7:30 PM **Banquet (Cape Florida Room, 316).**

Tuesday, 15 November 2005

Invited Talk 3 **Cape Florida Room (#316)**

8:45 AM *Combustion Challenges in Micro Turbines* ....
Jeffrey Willis, Capstone Turbine Corporation

Laminar Flames and Edge Flames (Key West Room, 218A)
Chair: Michael W. Renfro, University of Connecticut

9:45 AM *Propagating Edge Flame Response to Multiple Stoichiometric Gradients* ....
Stanislav Kostka Jr., William F. Carnell Jr., Michael W. Renfro, University of Connecticut

10:05 AM *Influence of Advective Heat Flux on Steady Negative Edge Flame Formation* ....
William F. Carnell Jr., Michael W. Renfro, University of Connecticut

10:25 AM *Experimental Measurements of Two-Dimensional Planar Propagating Edge Flames* ....
Marcos Villa-Gonzalez, Anthony Marchese, Rowan University, John W. Easton, Fletcher Miller, National Center for Space Exploration Research

10:45 AM **Break.**

11:05 AM *A Computational and Experimental Study of Transient Spherical Diffusion Flames in Microgravity* ....
Melissa K. Chernovsky, Songtao Tang, Hong G. Im, Arvind Atreya, University of Michigan

11:25 AM *Modeling of NOx Formation in Circular Laminar Jet Flames* ....
Vivek Siwatch, Texas A&M University

11:45 AM *Experimental and Computational Study of the Interaction between a Non-Premixed Methane Flame and Twin Vortices in the Axisymmetric Counterflow Geometry* ....
Giuliano Amantini, Yale University

Fire and Flame Suppression (Key West Room, 218B)
Chair: William Pitts, NIST

9:45 AM *CFD Modeling of Air Vitiation and Flame Extinction in Poorly Ventilated Compartment Fires* ....
Zhixin Hu, Yunyong Utiskul, James G. Quintiere, Arnaud Trouve, University of Maryland

10:05 AM *Application of Zone Models for Under-Ventilated Compartment Fires* ....
Vivien Lecoustre, ENSMA, Tensei Mizukami, Yunyong Utiskul, University of Maryland at College Park, James G. Quintiere, Arnaud Trouvé, University of Maryland

10:25 AM *Extinction of Vitiated Flame Sheets* ....
Justin Williamson, Andre W. Marshall, Arnaud Trouve, University of Maryland

10:45 AM **Break.**

11:05 AM *The Impact of Evaporation and Flow Behavior on the Suppression Effectiveness of sub-10-μm Water Drops in a Propane/Air Co-flow Non-Premixed Cup Burner Flame* ....
Brian T. Fisher, Andrew R. Awtry, James W. Fleming, Ronald S. Sheinson, Naval Research Laboratory

11:25 AM *Development of a Water-Mist Fire Suppression Tool for Low-Gravity Fire Suppression Modeling* ....
Douglas A. Schwer, K. Kailasanath, Naval Research Lab , Angel Abbud-Madrid, Center for Commercial Applications of Combustion in Space

11:45 AM *Large-Scale Particle Image Velocimetry Measurements of a Fire-Induced Doorway Flow* ....
Rodney A. Bryant, Erik L. Johnsson, Institute of Standards and Technology

Practical Combustors and Fuels (Key West Room, 218C)
Chair: Anthony Marchese, Rowan University

9:45 AM *Experimental Study on the Low-Temperature Ignition Behavior of Gas Turbine Fuel Blends* 181
Jaap De Vries, Eric L. Petersen, Joel M. Hall, Tony Amadio, Stefanie Simmons, University of Central Florida

10:05 AM *A Regenerative Multiple Flamelet Model for PPCI Engine Simulations* 185
Vasileios Hamosfakidis, Hong G. Im, Dennis N. Assanis, University of Michigan

10:25 AM *The Effect of DTBP on Gasoline and SI Primary Reference Fuels* 189
Rodney Johnson, Xiaohui Gong, Nicholas P. Cernansky, David L. Miller, Drexel University

10:45 AM **Break.**

11:05 AM *NOx Emission From Biodiesel Powered Vehicles During Realistic In-Use Driving Conditions* 193
Anthony Marchese, Robert Hesketh, Sarina Colligan, Andrew Toback, Rowan University, Amy Mensch, University of Maryland, Baltimore County

11:25 AM *Effect of Operating Frequency and Fill Time on PDE-Ejector Thrust Performance* 197
Robert J. Santoro, Rafat Shehadeh, Nicolas Bouvet, Seong-Young Lee, Sibtosh Pal

11:45 AM *Injector Placement Effects on Transverse Self-Induced Instabilities in a Multi-Element Rectangular Rocket Chamber* 201
William Marshall, Sibtosh Pal, Roger W. Woodward, Robert J. Santoro, Pennsylvania State University

Invited Talk 4 **Cape Florida Room (#316)**

1:30 PM *Recent Advances in Flame-Sampling Molecular-Beam Mass Spectrometry* 205
Phillip R. Westmoreland, University of Massachusetts Amherst

Measurements in Reacting Systems (Key West Room, 218A)
Chair: J. Houston Miller, George Washington University

2:30 PM *Simultaneous In-Situ Measurements of Temperature and Water Partial Pressure in a PEM Fuel Cell Under Steady and Dynamic Cycling Conditions* 213
Saptarshi Basu, Michael W. Renfro, Baki M. Cetegen, University of Connecticut

2:50 PM *Temporally Resolved Species Measurements from an Acoustically Forced Methane/Nitrogen Axi-Symmetric Flame Using Pulsed Quartz Microprobe Gas Extraction Followed by Electron Impact Mass Spectrometry* 217
Maria A. Puccio, Jennifer D. Herdman, J. Houston Miller, George Washington University, Blair C. Connelly, Mitchell D. Smooke, Marshall B. Long, Yale University

3:10 PM *Identification of Species and Separation of Isomers in a Premixed Fuel-Rich Cyclohexane Flame* 221
Saugata Gon, Matthew E. Law, Phillip R. Westmoreland, University of Massachusetts Amherst, Terrill A. Cool, Juan Wang, Cornell University , Nils Hansen, Craig A. Taatjes, Sandia National Laboratories, Tina Kasper, Patrick Oßwald, Universität Bielefeld

3:30 PM **Break.**

3:50 PM *Measurement of Soot Particle Size Distributions from a Well Stirred Reactor-Plug Flow Reactor* 225
David B. Lenhert, Samuel L. Manzello, Institute of Standards and Technology , Ahmet Yozgatligil, Michael R. Zachariah, University of Maryland College Park

4:10 PM *In-situ Measurements of Primary Particle Diameter and Structure of Soot in a Laminar Diffusion Flame* .....
Suresh S. Iyer, Thomas A Litzinger, Seong-Young Lee, Robert J. Santoro, Pennsylvania State University

4:30 PM *Silicon Carbide Filament-based Diagnostics in Oxygen Enhanced Flames* .....
Sravan Ravinutala, S.S. Krishnan, IUPUI , Peter B. Sunderland, University of Maryland Jay Gore, Purdue University

4:50 PM *Development of a Multi-Gas Analyzer Using Cavity Ringdown Spectroscopy for use in Fire Detection*.....
Eric A. Fallows, Brendan McAndrew, J. Houston Miller, George Washington University

Modeling of Laminar Flames (Key West Room, 218B)
Chair: Beth Anne V. Bennett, Yale University

2:30 PM *Importance of Chemical Kinetic Models on the Self-Excited Acoustic Response of Methane-Air Non-Premixed Counterflow Flames* .....
Andrea C. Zambon, Harsha K. Chelliah, University of Virginia

2:50 PM *A Mass-Conserving Vorticity-Velocity Formulation with Application to Axisymmetric Laminar Methane Flames*.....
Seth B. Dworkin, Beth Anne V. Bennett, Mitchell D. Smooke, Yale University

3:10 PM *Parallel Domain Decomposition Meshless Modeling of Dilute Chemical Species Transport*.....
Zaher El Zahab, Eduardo Divo, Alain Kassab, University of Central Florida

3:30 PM **Break.**

3:50 PM *Computational and Experimental Study of Axisymmetric Laminar Ethylene/Air Diffusion Flame Doped with Dimethyl Ether and Ethanol*.....
Beth Anne V. Bennett, Charles S. McEnally, Lisa D. Pfefferle, Mitchell D. Smooke, Yale University , Meredith B. Colket, UTRC

4:10 PM *Excess Air in Laminar Jet Flames and NOx Emission* .....
Vivek Siwatch, Kalyan Annamalai, Texas A&M University, Todd Tillman, ITT

4:30 PM *Fuel Stream and Air Stream CO_2 Dilution of Laminar Methane-Air Counterflow and Jet Flames*.....
Andrew Lock, Alejandro M. Briones, Suresh K. Aggarwal, University of Illinois at Chicago, Ishwar K. Puri, Virginia Polytechnic Institue and State University Uday Hegde, NASA Glenn Research Center

4:50 PM *Computational and Experimental Study of Molecular Growth in Forced, Time-Varying Flames* .....
Blair C. Connelly, Beth Anne V. Bennett, Seth Dworkin, Mitchell D. Smooke, Marshall B. Long, Yale University , J. Houston Miller, Maria A. Puccio, Jennifer D. Herdman, George Washington University

Novel Combustors and Heterogeneous Combustion (Key West Room, 218C)
Chair: Christopher Cadou, University of Maryland

2:30 PM *Acoustically Enhanced Radiant Combustion*.....
Rami Sabbah, Francisco Ruiz, Illinois Institute of Technology

2:50 PM *Investigation of Enhanced Stability in Micro-Combustors*.....
Timothy Leach, Ananthanarayanan Veeraragavan, Christopher Cadou, University of Maryland

3:10 PM *Evaluation of a Mechanism for Lean CH_4 Combustion on Pd Catalysts* .....
Seyed-A.S. Reihani, Gregory S. Jackson, University of Maryland , Timothy Griffin, University of Applied Sciences – Basel, Markus M. Wolf, Alstom Power Research Center

3:30 PM **Break.**

3:50 PM *From JP-8 to Electric Power Using Combustion at Small Scales and a Free Piston Stirling Engine to Replace Batteries*.....
Alessandro Gomez, Bruno Coriton, Yale Center for Combustion Studies, Jonathan Berry, Subir Roychoudhury, Precision Combustion Inc., James Huth, Sunpower, Inc.

4:10 PM *A Computational Study of the Reduction of Ceria (111), (110) and (100) Surfaces by H_2*.....
Hsin Tsung Chen, Y. M. Choi, Meilin Liu, Georgia Institute of Technology, M. C. Lin, Emory University

4:30 PM *Modeling Heterogeneous Combustion of Porous Carbon Particles* .....
Jared L. Kassebaum, Harsha K. Chelliah, University of Virginia

4:50 PM *Kinetics of OH Chemiluminescence in the Presence of Silicon*.....
Joel M. Hall, Eric L. Petersen, University of Central Florida