

Chemical and Physical Processes of Combustion

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

November 13-15, 2005
Orlando, Florida, USA

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Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571
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Monday, 14 November 2005

Invited Talk 1

1 Combustion Chemistry Models and Data: A New Paradigm for the 21st Century

William H. Green, MIT

Turbulence and Fire Topics: Special Talk on World TradeCenter

William L. Roberts, North Carolina State University

2 Micro-Vortex/Flame Interactions and Their Implications in Turbulent-Flame Modeling

Viswanath R. Katta, Terrence Meyer, Innovative Scientific Solutions, Inc, William Roquemore, Air Force Research Laboratory

6 A Comparison of Turbulent Premixed Combustion Models

Scott M. Martin, Siemens Power Corporation

10 Ignition of Vegetation and Mulch by Firebrands in Wildland/Urban Interface (WUI) Fires

Samuel L. Manzello, Thomas Cleary, John Shields, Jiann C. Yang, National Institute of Standards and Technology

11 Use of Visual Imagery for the NIST World Trade Center Investigation

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

Chemical Kinetics

Chair: Eric L. Petersen, University of Central Florida

15 Theoretical Study of the Kinetics and Mechanism for the Radical Reaction of $C_2H_5O_1$ with H

Kun Xu, Zhen Feng Xu, M. C. Lin, Department of Chemistry, Emory University

16 Ab Initio Kinetics for the Unimolecular Reaction $C_6H_5OH \rightarrow CO + C_5H_6$

Zhen Feng Xu, M. C. Lin, Department of Chemistry, Emory University

17 1,5-Hexadiyne and Fulvene Presence in Premixed Allene and Propyne Flames

Matthew E. Law, Saugata Gon, Phillip R. Westmoreland, University of Massachusetts Amherst, Terrill A. Cool, Juan Wang Cornell University, Nils Hansen, Sandia National Laboratories

21 Theoretical Study on the Reaction of CH_3OH with OH Radical

Shucheng Xu, M.C. Lin, Emory University

22 Theoretical Study Of Hydrogen Abstraction From Dimethyl Ether By OH Radical: Rate Constant Prediction

Shucheng Xu, M.C. Lin, Emory University

23 Kinetics of the Thermal Decomposition of t-Butyl-1,3-Cyclopentadiene: Ring Expansion and Radical Formation

W. Sean McGivern, Jeffrey A. Manion, Wing Tsang, National Institute of Standards and Technology

Ignition/Extinction

Chair: David L. Miller, Drexel University

27 Ignition Delay of Oxygenated Fuel Droplets

Matthew Hammill, Timothy Vaughn, Anthony Marchese, Rowan University

31 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

35 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

38 Lewis Number Effects on the Extinction of Counterflow Diffusion Flames

Marcos Chaos, Princeton University, Ruey-Hung Chen, University of Central Florida

42 Laser Ignition of Hydrogen Diffusion Jet Flame Diluted with Nitrogen

Phuoc X. Tran, Fredrick, P White, DOE/NETL

46 Computational Singular Perturbation Analysis of n-Heptane Two-Stage Ignition

Andrei Kazakov, Marcos Chaos, Zhenwei Zhao, Frederick L. Dryer, Princeton University

Invited Talk 2

50 Flame Synthesis of Nanostructured Materials

Stephen Tse, Rutgers University

Mechanisms and Reduced Mechanisms

Chair: W. Sean McGivern, NIST

54 Reduced High-Temperature Mechanisms for Large Paraffins - n - Hexadecane

Marcos Chaos, Andrei Kazakov, Zhenwei Zhao, Frederick L. Dryer, Princeton University, Stephen P. Zeppieri, Technologies Research Center

58 Application Of The ICE-PIC Method For The Dimension Reduction Of Chemical Kinetics

Zhuyin Ren, Stephen B. Pope, Cornell University

62 Obtaining Accurate Solutions Using Reduced Chemical Kinetic Models

William H. Green, O.O. Oluwole, MIT

64 Development of a Chemical Kinetics Mechanism for CH₄/H₂/Air Ignition at Elevated Pressures

Joel M. Hall, Eric L. Petersen, University of Central Florida

68 Insights Into a Premixed Stoichiometric Cyclohexane Flame

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

72 An Investigation of the Suppression Mechanism of CF₃Br Using the Reduced Kinetic Mechanisms for Premixed Hydrogen-Air-CF₃Br Flames

Zhuyin Ren, Stephen B. Pope, Cornell University

76 An Existing Global Heptane Mechanism Augmented with Diffusive Transport

Howard Pearlman, Michael Foster, Drexel University

Propellants and Detonations

Chair: Thomas A. Litzinger, The Pennsylvania State University

80 Confined Rapid Thermolysis/FTIR/ToF Studies of Imidazolium-based Ionic Liquids

Arindrajit Chowdhury, Stefan T. Thynell, Pennsylvania State University

84 Confined Rapid Thermolysis/FTIR/ToF Studies of Triazolium-based Ionic Liquids

Arindrajit Chowdhury, Stefan T. Thynell, Pennsylvania State University

88 Laser-driven Decomposition and Combustion of 4-Amino-1,2,4-Triazolium Nitrate

Jianquan Li, Thomas A. Litzinger, Pennsylvania State University

92 Impact of Nanoscale Aluminum on the Burn Rate of Composite Propellants Manufactured using Conventional Mixing Techniques

Alexander R. P. LePage, M. Stephens, University of Central Florida

96 Kinetics for the Combustion Initiation Reaction of Ammonium Perchlorate in the Condensed Phase

R. S. Zhu, M. C. Lin, Emory University

97 Curvature Effects On Detonations With Mole Decrement Reactions

Viktor Gorchkov, Mark Short, University of Illinois at Urbana-Champaign

101 Linear Stability Analysis of ZND Detonation Waves in General Reactive Systems

Charles B. Kiyanda, Mark. Short, University of Illinois at Urbana-Champaign

Soot

Chair: Baki Cetegan, University of Connecticut

105 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

109 The Effects of Dimethyl Ether and Ethanol on Benzene and Soot Formation in Ethylene Nonpremixed Flames

Charles S. McEnally, Lisa D. Pfefferle, Yale University

113 Soot Reduction by NO₂ 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

117 Soot Distributions in a Planar Diffusion Flame Wrapped by a Line Vortex

Saptarshi Basu, Baki M. Cetegen, University of Connecticut

121 Transient Dynamics Of Soot In Ethylene-Air Nonpremixed Counterflow Flames

Chun Sang Yoo, Hong G. Im, University of Michigan

125 Are the Fractal Characteristics of Soot Constant?

Suresh S. Iyer, Thomas A Litzinger, Robert J Santoro, Pennsylvania State University

129 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

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Jeff Willis, Capstone Turbine Corporation

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Chair: William Pitts, NIST

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Vivien Lecoustre, ENSMA, Tensei Mizukami, Yunyong Utiskul, University of Maryland at College Park, James G. Quintiere, Arnaud Trouvé, University of Maryland

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Justin Williamson, Andre W. Marshall, Arnaud Trouve, University of Maryland

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Brian T. Fisher, Andrew R. Awtry, James W. Fleming, Ronald S. Sheinson, Naval Research Laboratory

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Douglas A. Schwer, K. Kailasanath, Naval Research Lab , Angel Abbud-Madrid, Center for Commercial Applications of Combustion in Space

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Rodney A. Bryant, Erik L. Johnsson, Institute of Standards and Technology

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Chair: Michael Renfro, , University of Connecticut

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Stanislav Kostka Jr., William F. Carnell Jr., Michael W. Renfro, University of Connecticut

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William F. Carnell Jr., Michael W. Renfro, University of Connecticut

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Marcos Villa-Gonzalez, Anthony Marchese, Rowan University, John W. Easton, Fletcher Miller, National Center for Space Exploration Research

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Melissa K. Chernovsky, Songtao Tang, Hong G. Im, Arvind Atreya, University of Michigan

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Vivek Siwatch, Texas A&M University

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Giuliano Amantini, Yale University

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Jaap De Vries, Eric L. Petersen, Joel M. Hall, Tony Amadio, Stefanie Simmons, University of Central Florida

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Vasileios Hamosfakidis, Hong G. Im, Dennis N. Assanis, University of Michigan

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Rodney Johnson, Xiaohui Gong, Nicholas P. Cernansky, David L. Miller, Drexel University

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Anthony Marchese, Robert Hesketh, Sarina Colligan, Andrew Toback, Rowan University, Amy Mensch, University of Maryland, Baltimore County

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Robert J. Santoro, Rafat Shehadeh, Nicolas Bouvet, Seong-Young Lee, Sibtos Pal, Pennsylvania State University

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William Marshall, Sibtos Pal, Roger W. Woodward, Robert J. Santoro, Pennsylvania State University

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Phillip R. Westmoreland, University of Massachusetts Amherst

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Chair: J. Houston Miller, George Washington University

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Saptarshi Basu, Michael W. Renfro, Baki M. Cetegen, University of Connecticut

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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

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Suresh S. Iyer, Thomas A Litzinger, Seong-Young Lee, Robert J. Santoro, Pennsylvania State University

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Rami Sabbah, Francisco Ruiz, Illinois Institute of Technology

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Jared L. Kassebaum, Harsha K. Chelliah, University of Virginia

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