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

Printed from CD-ROM with permission by:
Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571
www.proceedings.com
CSIN: 9999900108
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 Trade Center
William L. Roberts, North Carolina State University

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

6 A Comparison of Turbulent Premixed Combustion Models
Scott M. Martin, Siemens Power Corporation

10 Ignition of Vegetation and Mulch by Firebrands in Wildland/Urb... 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\textsubscript{2}H\textsubscript{5}O\textsubscript{4} with H
Kun Xu, Zhen Feng Xu, M. C. Lin, Department of Chemistry, Emory University

16 Ab Initio Kinetics for the Unimolecular Reaction C\textsubscript{6}H\textsubscript{5}OH + CO + C\textsubscript{5}H\textsubscript{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\textsubscript{3}OH 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

Tuesday, 15 November 2005

Invited Talk 3
133 Combustion Challenges in Micro Turbines
Jeff Willis, Capstone Turbine Corporation

Fire and Flame Supression
Chair: William Pitts, NIST

134 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

138 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

142 Extinction of Vitiated Flame Sheets
Justin Williamson, Andre W. Marshall, Arnaud Trouve, University of Maryland

146 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
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

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

Laminar Flames and Edge Flames
Chair: Michael Renfro, University of Connecticut

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

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

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

A Computational and Experimental Study of Transient Spherical Diffusion Flame in Microgravity
Melissa K. Chernovsky, Songtao Tang, Hong G. Im, Arvind Atreya, University of Michigan

Modeling of NO\textsubscript{x} Formation in Circular Laminar Jet Flames
Vivek Siwatch, Texas A&M University

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

Practical Combustors and Fuels
Chair: Anthony Marchese, Rowan University

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

A Regenerative Multiple Flamelet Model for PPCI Engine Simulations
Vasileios Hamosfakidis, Hong G. Im, Dennis N. Assanis, University of Michigan

The Effect of DTBP on Gasoline and SI Primary Reference Fuels
Rodney Johnson, Xiaohui Gong, Nicholas P. Cemansky, David L. Miller, Drexel University

NO\textsubscript{x} Emission From Biodiesel Powered Vehicles During Realistic In-Use Driving Conditions
Anthony Marchese, Robert Hesketh, Sarina Colligan, Andrew Toback, Rowan University, Amy Mensch, University of Maryland, Baltimore County

Effect of Operating Frequency and Fill Time on PDE-Ejector Thrust Performance
Robert J. Santoro, Rafat Shehadeh, Nicolas Bouvet, Seong-Young Lee, Sibtosh Pal, Pennsylvania State University
201 Injector Placement Effects on Transverse Self-Induced Instabilities in a Multi-Element Rectangular Rocket Chamber

Invited Talk 4

205 Recent Advances in Flame-Samples Molecular-Beam Mass Spectrometry
Phillip R. Westmoreland, University of Massachusetts Amherst

Measurements in Reacting Systems
Chair: J. Houston Miller, George Washington University

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

217 Temporally Resolved Species Measurements from an Acoustically Forced Methane/Nitrogen Axisymmetric Flame Using Pulsed Quartz Microprobe GasExtraction Followed by Electron Impact Mass Spectrometry
Maria A. Puccio, Jennifer D. Herdman, J. Houston Miller, George Washington University, Blair C. Connelly, Mitchell D. Smooke, Marshall B. Long, Yale University

221 Identification of Species and Separation of Isomers in a Premixed Fuel-Rich Cyclohexane Flame
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

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

226 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

230 Silicon Carbide Filament-based Diagnostics in Oxygen Enhanced Flames
Sravan Ravinutala, S.S. Krishnan, IUPUI, Peter B. Sunderland, University of Maryland, Jay P. Gore, Purdue University

231 Development of a Multi-Gas Analyzer Using Cavity Ring down Spectroscopy for use in Fire Detection
Eric A. Fallows, Brendan McAndrew, J. Houston Miller, George Washington University

Modeling of Laminar Flames
Chair: Beth Bennett, Yale University

235 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

239 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
243 Parallel Domain Decomposition Meshless Modeling of Dilute Chemical Species Transport
Zaher El Zahab, Eduardo Divo, Alain Kassab, University of Central Florida

247 Computational and Experimental Study of Axisymmetric Laminar Ethylene/Air Diffusion Flames 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

251 Excess Air in Laminar Jet Flames and NO\textsubscript{x} Emission
Vivek Siwatch, Kalyan Annamalai, Texas A&M University, Todd Tillman, ITT

255 Fuel Stream and Air Stream CO\textsubscript{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 Institute and State University Uday Hegde, NASA Glenn Research Center

259 Computational and Experimental Study of Molecular Growth in Forced, Time-Varying Flames
Blair Blair 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**
Chair: Christopher Cadou, University of Maryland

263 Acoustically Enhanced Radiant Combustion
Rami Sabbah, Francisco Ruiz, Illinois Institute of Technology

264 Investigation of Enhanced Stability in Micro-Combustors
Timothy Leach, Ananthanarayanan Veeraragavan, Christopher Cadou, University of Maryland

268 Evaluation of a Mechanism for Lean CH\textsubscript{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

272 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.

276 A Computational Study of the Reduction of Ceria (111), (110) and (100) Surfaces by H\textsubscript{2}
Hsin Tsung Chen, Y. M. Choi, Meilin Liu, Georgia Institute of Technology, M. C. Lin, Emory University

277 Modeling Heterogeneous Combustion of Porous Carbon Particles
Jared L. Kassebaum, Harsha K. Chelliah, University of Virginia

281 Kinetics of OH Chemiluminescence in the Presence of Silicon
Joel M. Hall, Eric L. Petersen, University of Central Florida