

Combustion Institute

Fall Technical Meeting of the Eastern States Section of the Combustion Institute 2007

“Chemical and Physical Processes in Combustion”

October 21-24, 2007
Charlottesville, Virginia, USA

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571
www.proceedings.com

ISBN: 978-1-60423-945-4

Some format issues inherent in the e-media version may also appear in this print version.

Combustion Institute
Fall Technical Meeting of the Eastern
States Section of the Combustion Institute
2007

TABLE OF CONTENTS

Modeling Wildland and Wildland-Urban Interface Fires	1
<i>W. Mell</i>	
Theoretical Study of the Combustion and Thermal Decomposition of RDX Part I: Kinetic Modeling - Part II: Detailed Kinetics on Initial Reaction Paths.....	3
<i>W. Anderson, G. Da Silva, J. Bozzelli, C. Conner</i>	
Chemically Activated Oxidation of N-Propyl Radicals.....	17
<i>W. Tsang</i>	
Ab Initio Chemical Kinetics for N₂ Reaction with Singlet and Triplet CH₂ Radicals	22
<i>S. Xu, M. Lin</i>	
New Shock-Tube Facility for Studies in Chemical Kinetics at Engine Conditions	26
<i>C. Aul, J. De Vries, E. Petersen</i>	
Preignition Oxidation Chemistry of n-Decane	32
<i>M. Kurman, R. Natelson, N. Cernansky, D. Miller</i>	
Molecular Dynamics Study of C-C Bond Dissociation in Linear Alkanes and Polyethylene: Effects of Condensed Phase.....	39
<i>K. Popov, V. Knyazev</i>	
Methane and Dimethyl Ether Oxidation at Elevated Temperatures and Pressures.....	44
<i>C. Zinner, E. Petersen</i>	
Rate-Controlled Constrained-Equilibrium Calculations of the Combustion Products in the Expansion Stroke of an Internal Combustion Engine	48
<i>M. Janbozorgi, D. Goldthwaite, H. Metghalchi, J. Keck</i>	
Transported PDF Modeling for a Direct-Injection PCCI Engine	57
<i>E. Kung, D. Haworth</i>	
A Computational Fluid Dynamics Study of a Rapid Compression Machine	66
<i>G. Mittal, M. Raju, C. Sung, K. Kundu</i>	
A Rapid Compression Machine Study of Dimethyl Ether Autoignition.....	74
<i>G. Mittal, M. Chaos, C. Sung, F. Dryer</i>	
Shock-tube Study of the Ignition Delay Times of Ethanol at High Pressures and Intermediates Temperatures Experimental and Numerical Approaches	82
<i>M. Fikri, L. Cancino, A. Oliveira, C. Schulz</i>	
The Kinetics and Mechanism for the Unimolecular Decomposition of Acetophenone: Ab Initio MO and VTST/RRKM Calculations.....	88
<i>S. Ju, H. Chen, M. Lin, J. Chang, M. Weng</i>	
Measurements of HCN and C₂H₂ from a Pyridine-Doped Methane/Air Axisymmetric Flame Using Cavity Ringdown Spectroscopy.....	93
<i>E. Fallows, M. Puccio, J. Houston-Miller</i>	

Chain Branching and Termination Paths in Oxidation of n-alkanes: Comprehensive Complete Basis Set-QB3 Study on the Association of n-pentyl Radical with O₂, Isomerization and Addition of Second Oxygen Molecule.....	99
<i>R. Asatryan, J. Bozzelli</i>	
The High Pressure Combustion of Saturated and Unsaturated C₇ Hydrocarbons	105
<i>S. Garner, R. Sivaramakrishnan, K. Brezinsky, P. Dagaut</i>	
Thermochemistry and Kinetics of the α-hydroxyethyl Radical + O₂ Reaction in Ethanol Combustion.....	114
<i>G. Da Silva, L. Liang, J. Bozzelli, J. Farrell</i>	
Flow Reactor Pyrolysis of Diethyl Sulfide	129
<i>X. Zheng, E. Fisher, F. Gouldin, L. Zhu, J. Bozzelli</i>	
Combustion in an Optical Diesel Engine Fueled with Diesel and Bio-Diesel Fuels Using Multiple Injection Strategies	145
<i>T. Fang, C. Lee</i>	
High Efficiency Residual Oil (SuperHERO) Gun for Liquid Waste Incineration	159
<i>I. Chung, J. Colannino</i>	
Intensity and Efficiency of Polydispersed Spray Fuel-Fed Well-Mixed Combustors	169
<i>D. Rosner, M. Arias-Zugasti, M. Labosky</i>	
A New Detailed Numerical Model of Isolated Droplet Combustion	172
<i>K. Kroenlein, A. Kazakov, F. Dryer</i>	
Confined Rapid Thermolysis/FTIR Spectroscopy/ToF Mass Spectrometry of TAGzT	181
<i>A. Chowdhury, S. Thynell</i>	
Optimization of Combustion Application Codes using Sparse Matrix Techniques.....	187
<i>M. Faju, C. Sung</i>	
Integrating Sensitivity Analysis into Directed Relation Graph with Error Propagation for Effective Chemical Mechanism Reduction.....	193
<i>M. Raju, C. Sung, K. Kundu</i>	
Error control of Model Reduction by Linearized Quasi Steady State Approximation	200
<i>X. Dong, W. Green</i>	
Ab Initio Chemical Kinetics and Mechanism for the CH₃O + O ^(3P) Reaction	206
<i>Z. Xu, M. Lin</i>	
Kinetic Modeling of the Benzyl + HO₂ Reaction.....	212
<i>G. Da Silva, J. Bozzelli</i>	
Sensitivity Analysis for the Thermal Gas Phase Reactions of 5-Methyl-Hexyl Radicals	218
<i>I. Awan, W. Tsang, W. McGivern, J. Manion</i>	
Experimental Investigation of Kinetic Ignition of Counterflow Diffusion Flames by Plasma-Activated Ultra-Lean Premixtures	226
<i>T. Ombrello, Y. Ju</i>	
Modeling of Carbon Nanotube Growth by Flame Synthesis	232
<i>S. Naha, I. Puri</i>	
Electrostatic Self-Assembly of a Nanoscale Thermite System into Ordered Microspheres	241
<i>J. Malchi, R. Yetter, T. Foley</i>	

Development and Preliminary Testing of an Electrolytic Ignition Microthruster for Space Propulsion.....	246
<i>M. Wu, R. Yetter</i>	
A Chemical Process for Converting Lipids to Transportation Fuels	250
<i>T. Turner, W. Roberts, L. Stikeleather</i>	
A Study of Emissions from Diesel and Vegetable Oile Fueled Vehicles.....	259
<i>T. Bockus, J. Mertens</i>	
Study of Reaction Rates Through A Local Extinction Point in NonPremixed Flames	266
<i>W. Carnell Jr., M. Renfro</i>	
A Simple Model for a Small Wick Flame	273
<i>H. Baum</i>	
Computational and Experimental Study of Oxygen-enhanced Azisymmetric Laminar Methane Flames	282
<i>B. Bennett, Z. Cheng, R. Pitz, M. Smooke</i>	
Effects of Ethylene Addition on Counterflow Ignition and Flame Propagation in Methane/Ethylene Mixtures.....	290
<i>W. Liu, Y. Huang, T. Lu, D. Zhu, C. Law</i>	
Nonlinear Effects in the Experimental Determination of Laminar Flame Properties from Stretched Flames	296
<i>A. Kelley, C. Law</i>	
Structure of Fuel/Oxygen/Diluent (Argon, Helium, Nitrogen) Premixed Flames at High Pressures and Temperatures	305
<i>K. Far, R. Andrews, F. Parsinejad, H. Metghalchi</i>	
The Structure of a JP-8 Counterflow Diffusion Flame by Gas Sampling and GC/MS Analysis.....	311
<i>L. Tosatto, B. La Mantia, P. Duchaine, M. Smooke, A. Gomez</i>	
Soot Topography in a Planar Diffusion Flame Wrapped by Interacting Line Vortices	316
<i>S. Basu, S. Chaudhuri, B. Cetegen</i>	
Assessment of RANS-Based Turbulent Combustion Models for Prediction of Gas Turbine Emissions: Turbulence Model and Reaction Mechanism Effects	321
<i>J. Nanduri, I. Celik, P. Strakey, D. Parsons</i>	
Instantaneous Flamelet Displacement Speed Measurements on a Premixed Turbulent V-Flame.....	332
<i>S. Sattler, F. Gouldin</i>	
PDF Modeling of Turbulent Lean Premixed Combustion	338
<i>S. Yilmaz, P. Givi, P. Strakey</i>	
Effects of Spatial Mixture Gradients on Stabilization Zone Temperatures of Bluff-Body Stabilized Turbulent Premixed Conical Flames	342
<i>S. Chaudhuri, B. Cetegen</i>	
Temperature Measurements in the Stabilization Zone of Acoustically Modulated, Turbulent Premixed Conical Flames by Emission Spectroscopy	347
<i>S. Chaudhuri, B. Cetegen</i>	
Radiation-driven Flame Weakening Effects in Sooting Turbulent Diffusion Flames	354
<i>P. Narayanan, A. Trouve</i>	

Response of Premixed Flames to Equivalence Ration Oscillations: Non-Quasi Steady Effects	360
<i>Shreekrishna, T. Lieuwen</i>	
Auto-Ignition of Homogeneous Hydrogen/Air Mixture Subjected to Unsteady Temperature Fluctuations	373
<i>G. Bansal, H. Im, S. Lee</i>	
Predicting Dynamic Heat Release Rate in Turbulent Flames with Reduced-Order Models	382
<i>C. Martin, J. Ranalli, P. Black, W. Baumann, U. Vandsburger, R. West</i>	
Numerical Investigation of Acoustic Wave Interaction with 2D Counterflow Flames	396
<i>A. Sriram, H. Chelliah</i>	
The Stretch Effect on the Accurate Determination of Laminar Flame Speed using Expanding Flames in a Spherical Bomb.....	403
<i>Z. Chen, Y. Ju</i>	
Calculated Extinction Strain Rates for Binary Fuel Mixtures	411
<i>O. Park, E. Fisher</i>	
Laminar Flame Speeds of H₂/CO/O₂/He Mixtures at Elevated Pressure and Preheat Temperature	418
<i>J. Natarajan, Y. Kochar, T. Lieuwen, J. Seitzman</i>	
Quenching Limits of Hydrogen Diffusion Flames	427
<i>M. Butler, C. Moran, P. Sunderland, R. Axelbaum</i>	
A Paradigm Shift in the Interaction of Experiments and Computations in Combustion Research	435
<i>B. Connelly, B. Bennett, M. Smooke, M. Long</i>	
Stretch Effects on the Stability of Spherical Premixed Flames	445
<i>G. Jomaas, C. Law</i>	
Effect of Cylindrical Confinement on the Evolution of Outwardly Propagating Flames	450
<i>M. Burke, Y. Ju, F. Dryer</i>	
Evolved Combustion Products from CNT-Polymer Composites	459
<i>R. Vander Wal, J. Fujiyama-Novak, V. Pushkarev</i>	
Numerical Modeling of Two-Dimensional Smolder Structure	465
<i>A. Dodd, C. Lautenberger, A. Fernandez-Pello</i>	
Three-Dimensional Simulation of Suppression of Flames by Water-Mist Injection	475
<i>D. Schwer, K. Kailasanath</i>	
Experimental Comparison of Opposed and Concurrent Flame Spread in a Forced Convective Microgravity Environment	481
<i>S. Olson, F. Miller</i>	
Limiting Length and Non-growing Flames in Concurrent Flow over Thick Solids.....	485
<i>Y. Tseng, J. T'len</i>	
Promotion of Hydrogen-Air Ignition by Iron Compounds	493
<i>G. Linteris</i>	
Radiative Pyrolysis of JA2 from an Electrochemical Plasma Discharge.....	503
<i>M. Das, A. Choudhury, S. Thynell</i>	

Sooting Tendencies of Nonvolatile Aromatic Hydrocarbons.....	510
<i>C. McEnally, L. Pfefferle</i>	
Laminar Smoke Points of Waxes	519
<i>K. Allan, J. Kaminski, J. Bertrand, J. Head, P. Sunderland</i>	
The Impact of Detailed Multicomponent Transport and Thermal Diffusion Effects on Soot Formation in Ethylene/Air Flames	530
<i>S. Dworkin, M. Smooke, V. Giovangigli</i>	
Modeling the Effect of Flame Structure on the Formation of Aromatics in Opposed Flow Diffusion Flames	539
<i>S. Skeen, R. Axelbaum</i>	
Effects of C/O Ratio and Scalar Dissipation Rate on Sooting Limits of Spherical Nonpremixed Flames.....	547
<i>V. Lecoustre, B. Chao, P. Sunderland, D. Urban, D. Stocker, R. Axelbaum</i>	
Evidence for Polynuclear Aromatic Hydrocarbon Aggregation in Flames: Intermolecular Potential Calculations.....	557
<i>J. Herdman, J. Miller</i>	
Size Resolved Kinetics of Nickel Nanoparticle Oxidation by Ion-Mobility Classification.....	563
<i>L. Zhou, A. Rai, N. Piekiel, X. Ma, M. Zachariah</i>	
High Pressure Shock Tube Studies on C_(s)+CO₂	570
<i>B. Culbertson, R. Sivaramakrishnan, K. Brezinsky</i>	
On the Modelling of Porous Carbon Particle Combustion	576
<i>J. Kassebaum, H. Chelliah, F. Miller</i>	
Influences of Temperature and Available Carbon Sources on Synthesis of Carbon Nanotubes in Methane-Air Diffusion Flames	582
<i>T. Li, K. Kuwana, K. Saito, H. Zhang, Z. Chen</i>	
Deflagrations of Nitromethane and Nanoaluminum Mixtures	588
<i>J. Sabourin, R. Yetter, B. Asay, G. Risha, S. Son</i>	
Dependence of the Combustion Velocity on Particle Size and Pressure for an Al/CuO Thermite	595
<i>M. Weismiller, J. Malchi, R. Yetter, T. Foley</i>	
Effects of Dioctyl Sulfosuccinate on the Burning Rate of HTPB/AP Solid Composite Propellants	601
<i>M. Stephens, D. Reid, G. Carro, A. Lepage, S. Seal, E. Petersen</i>	
A First-Principles Study on the Sublimation/Decomposition of NH₄ClO₄.....	605
<i>R. Zhu, M. Lin</i>	
Single-walled Carbon Nanotube Growth from Composite Catalysts in Diffusion Flames	610
<i>C. Unrau, R. Axelbaum</i>	
Effects of Heat Loss on a Stagnation-Point Flow Catalytic Combustor	615
<i>J. Li, H. Im, J. Wiswall, M. Wooldridge</i>	
Upstream Flame Propagation in Catalytic Palladium and Platinum Microtubes.....	622
<i>M. Johnston, F. Miller, D. Dietrich, P. Struk, J. T'len</i>	
Role of the Knudsen Layer in Determining Surface Reaction Rates Based on Sticking Coefficients.....	628
<i>P. Zheng, C. Law</i>	

Turbulent Combustion Velocimetry in a Scramjet	632
<i>C. Smith, C. Goyne</i>	
Effects of Coaxial Air on Nitrogen-Diluted Hydrogen Jet Diffusion Flame Length and NO_x Emission	641
<i>N. Weiland, R. Chen, P. Strakey</i>	
Simultaneous 2-I OH Thermometry and PIV of Unsteady Methane-Air Kernel- Vortex Interactions.....	651
<i>S. Danby, W. Roberts</i>	
Effects of the Leading-Edge Reaction Zone on Lifted Flame Oscillations	658
<i>N. Moore, K. Lyons</i>	
Composition PDF/Method of Moments Modeling of Soot Formation in a Turbulent Ethylene/Air Jet Flame.....	664
<i>R. Mehta, D. Haworth, M. Modest</i>	
Three Dimensional Numerical Simulation of Flames Supported by a Spinning Porous-Plug Burner	670
<i>K. Hossain, T. Jackson, J. Buckmaster</i>	
Supersonic Combustion Research at NASA.....	674
<i>J. Drummond, P. Danehy, D. Bivolaru, R. Gaffney, S. Tedder, A. Cutler</i>	
Computational and Experimental Study of Coflow Diffusion Flames	686
<i>M. Smooke, M. Long, B. Connelly, M. Colket, R. Hall</i>	

Author Index