

Fall Technical Meeting of the Eastern States Section of the Combustion Institute 2011

**Storrs, Connecticut, USA
9-12 October 2011**

ISBN: 978-1-62276-125-8

Printed from e-media with permission by:

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



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

Copyright© (2011) by The Combustion Institute
All rights reserved.

Printed by Curran Associates, Inc. (2012)

For permission requests, please contact The Combustion Institute
at the address below.

The Combustion Institute
5001 Baum Boulevard
Suite 635
Pittsburgh, PA 15213-1851, USA

Phone: (412) 687-1366
Fax: (412) 687-0340

office@combustioninstitute.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2634
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

A-1: REACTION KINETICS I

A-01 Comparative Investigation of the High Pressure Autoignition of the Butanol Isomers	1
<i>Bryan Weber, Chih-Jen Sung</i>	
A-02 Ab Initio Kinetics for the Decomposition of α-Hydroxybutyl Radicals of n-Butanol	5
<i>Peng Zhang, Stephen Klippenstein, Chung K. Law</i>	
A-03 Water Elimination Rate Measurements for Tertiary-Butanol	14
<i>Joshua Heyne, Stephen Dooley, Frederick L. Dryer</i>	
A-04 Shock Tube Studies on the Decomposition of 2-Butanol	21
<i>Claudette Rosado-Reyes, Wing Tsang</i>	
A-05 High Pressure Study of 1,3,5-Trimethylbenzene Oxidation	27
<i>Soumya Gudiyella, Kenneth Brezinsky</i>	
A-06 Autoignition of Selected Alkyl-benzenes in a Rapid Compression Machine	33
<i>Kamal Kumar, Chih-Jen Sung</i>	

SESSION A-2: REACTION KINETICS II

A-08 Kinetics of H Atom Attack on Unsaturated Hydrocarbons Using Spectral Uncertainty Propagation and Minimization Techniques	38
<i>David Sheen, Claudette Rosado-Reyes, Wing Tsang</i>	
A-09 Methodology to Account for Multi-stage Ignition Events During Simulations of RCM Experiments	44
<i>S. Scott Goldsborough, Gaurav Mittal, Colin Banyon</i>	
A-10 Experimental and Surrogate Modeling Study of Gasoline Ignition in a Rapid Compression Machine	54
<i>Goutham Kukkadapu, Kamal Kumar, Chih-Jen Sung, Marco Mehl, W. J. Pitz</i>	
A-11 Emulating the Combustion Behavior of Real Jet Aviation Fuels by Surrogate Mixtures from Solvent Blends	58
<i>Saeed Jahangirian, Stephen Dooley, Venkatesh Iyer, Thomas A. Litzinger, Robert J. Santoro, Frederick L. Dryer</i>	
A-12 A Theoretical Study of H-abstraction Reactions of Monomethylhydrazine by OH Radical	73
<i>Hongyan Sun, Peng Zhang, Chung K. Law</i>	
A-13 Ab Initio Multireference Study of the Reactions of $\text{CH}_3\text{N}\cdot\text{NH}_2 + \text{OH}$	79
<i>Hongyan Sun, Chung K. Law</i>	
A-14 Chemical Activation and Thermal Reactions at Higher Temperatures	84
<i>Wing Tsang</i>	
A-15 Stoichiometric Effects on Oxidation and Benzene-Formation Chemistry in Premixed 1-Hexene Flames	88
<i>Wenjun Li, Phillip R. Westmoreland, Bin Yang, Nils Hansen</i>	

SESSION A-3: REACTION KINETICS III

A-16 Experimental and Theoretical Study on the Reactions of CHF Radicals with C_2H_2, C_2H_4 and NO in the Temperature Range of 296–670 K	92
<i>Xueliang Yang, Congxiang Chen, Phillip Westmoreland</i>	
A-17 Thermochemical Properties of Hydrofluorocarbons	97
<i>Eugene Paulechka, Kenneth Kroenlein, Andrei Kazakov</i>	
A-18 A High Temperature Model for the Combustion of Methylbutanoate	101
<i>Raghu Sivaramakrishnan, Wei Liu, Michael J. Davis, Sibendu Som, Douglas E. Longman</i>	
A-19 Density Functional Theory Study of the Ignition Mechanism of 2-Azido-N, N-Dimethylethanamine (DMAZ)	109
<i>Peng Zhang, Chung K. Law</i>	
A-20 Reaction Kinetics for TMEDA Combustion with Red Fuming Nitric Acid	114
<i>Nicole J. Labbe, Phillip R. Westmoreland</i>	

A-21 Metal Oxide Oxygen Carriers in Chemical Looping Combustion of Carbon: Evidence for Condensed Phase Reaction	119
<i>Nicholas Piekiet, Garth Egan, Michael Zachariah</i>	
A-22 Probing Oxygen Release Kinetics of Nanosized Metal Oxides by Temperature-Jump Time of Flight Mass Spectrometry	126
<i>Guoqiang Jian, Lei Zhou, Nicholas Piekiet, Michael Zachariah</i>	

SESSION A-4: REACTION KINETICS IV

A-23 Analysis of Chemical and Physical Processes During Pyrolysis of a Single Cylinder of Poplar Wood in Flow Reactor	132
<i>Hayat Bennadji, Elizabeth M. Fisher, Shaka Velaphi Shabangu, Krystle Smith</i>	
A-24 Experimental and Modeling Study of 2-Methylheptane Oxidation in a Flow Reactor, Shock Tube, and Rapid Compression Machine	136
<i>Saeed Jahangirian, D. Healy, S. Mani Sarathy, Stephen Dooley, Marco Mehl, William J. Pitz, Frederick L. Dryer, Henry J. Curran, Charles K. Westbrook</i>	
A-25 1,3,5-TriMethyl Benzene: Laminar Flame Speeds Measurements and Kinetic Modeling	150
<i>Pascal Dievart, Hwan Ho Kim, Stephen Dooley, Sang Hee Won, Yiguang Ju</i>	
A-26 An Updated Combustion Kinetic Model for Syngas Fuels and C₁ Oxygenates	156
<i>F. M. Haas, Sijm Vranckx, Marcos Chaos, Ravi X. Fernandes, Frederick L. Dryer</i>	
A-27 Rate Coefficients for H + O₂ + CO₂ → HO₂ + CO₂ Determined in a New High Pressure Laminar Flow Reactor	164
<i>F. M. Haas, Tanvir I. Farouk, Marcos Chaos, Michael P. Burke, Frederick L. Dryer</i>	
A-28 Extinction Limits of Non-premixed Counterflow Hydrogen/Oxygen/Nitrogen Flames: Comparison Between Experiments and Predictions with Kinetic and Transport Uncertainties	171
<i>Gaetano Esposito, Brendyn G. Sarnacki, Harsha K. Chelliah</i>	

SESSION A-5: REACTION KINETICS V

A-29 Efficient Development of Accurate Detailed Combustion Chemistry Models	179
<i>William H. Green</i>	
A-30 A Multi-scale Approach to Model Development	183
<i>Michael P. Burke, Stephen J. Klippenstein, Lawrence B. Harding</i>	
A-31 Parallel Computation of Chemical Mechanism Reduction	189
<i>Mandhapati P. Raju, Mingjie Wang</i>	
A-32 Computationally-efficient Parallel Implementation of Combustion Chemistry in LES/PDF Computations	197
<i>Varun Hiremath, Steven R. Lantz, Haifeng Wang, Stephen B. Pope</i>	
A-33 Development of a Detailed Zero- and One-dimensional Aromatic and Cyclo-C₅ Model	207
<i>Ryan Closson, Vik Gill, Adam Hashemi, Yelena Kozachkova, Thomas Tshkoff, Yevgeniy Tsypin, Robert G. Butler</i>	
A-34 Elementary-reaction Kinetics of Glucose Pyrolysis	212
<i>Vikram Seshadri, Jordan R. Keith, Phillip R. Westmoreland</i>	

B-1: PISTON AND GAS TURBINE ENGINES

B-01 Hydrocarbon Fingerprint in Gas Turbine Emissions	216
<i>Stephen Zeppieri, Meredith B. Colket</i>	
B-02 Extended Kernel Lifetimes During Altitude Relight	222
<i>Meredith B. Colket, Stephen Zeppieri, Heidi Hollick, Shiling Zhang</i>	
B-03 Response of Non-premixed Flames to Bulk Flow Perturbations	229
<i>Nicholas Magina, Vishal Acharya, Timothy Lieuwen</i>	
B-04 Three Dimensional Simulations of Diesel Sprays Using N-Dodecane As a Surrogate	241
<i>Sibendu Som, Douglas E. Longman, Zhaoyu Luo, Max Plomer, Tianfeng Lu</i>	
B-05 Thermodynamics of a Rotating Detonation Engine with Micro-Injectors	255
<i>Douglas A. Schwer, Kailas Kailasanath</i>	
B-06 Thermodynamics of Rotating Detonation Performance	269
<i>Craig A. Nordeen, D. Schwer, F. Schauer, J. Hoke, T. Barber, B. M. Cetegen</i>	

SESSION B-2: SOOT

B-08 Combustion Particulate Detection and Analysis Via a Micro-glow Discharge	283
<i>Chethan K. Gaddam, Ganesh R. Bhimanapati, Amrita Mukherjee, Jane H. F. Novak, Randy L. Vander Wal, Benjamin Ward</i>	
B-09 Quantification of Hydrocarbon Condensation on Combustion Soot Particles	288
<i>David Liscinsky, Zhenhong Yu, Scott Herndon, Jon Franklin, Jay Peck, Hsi-Wu Wong, Mina Jun, Ian Waitz, Archer Jennings, Bruce True, Meredith B. Colket, R. Miake-Lye</i>	
B-10 Molecular-weight Growth in Fuel-rich Toluene + Methane and Toluene + Acetylene Flames	295
<i>Wenjun Li, Phillip R. Westmoreland, Bin Yang, Nils Hansen</i>	
B-11 XPS & HRTEM Characterization of PM	300
<i>R. L. Vander Wal, V. Bryg, M. D. Hays</i>	
B-12 Effects of M-xylene, Dodecane and JP-8 Addition on Soot in Laminar, N₂-diluted Ethylene Coflow Diffusion Flames from 1 to 5 Atm	304
<i>Anne G. Mouis, Venkatesh R. Iyer, Milton J. Linevsky, Thomas A. Litzinger, Robert J. Santoro</i>	
B-13 Comparison of Sooting Propensity of JP-8 with Its Surrogates in a Wick Burner and a Model Gas Turbine Combustor	311
<i>Venkatesh Iyer, Suresh Iyer, Stephen Dooley, Milton Linevsky, Frederick Dryer, Thomas Litzinger, Christopher Mordaunt, Robert Santoro</i>	
B-14 Sooting Formation from Oxygenated Hydrocarbons	318
<i>Charles S. McEnally, Lisa D. Pfefferle</i>	
B-15 Experimental and Numerical Study of JP-8 Coflow Flames	325
<i>Luca Tosatto, Federico Mella, Beth Anne V. Bennett, Marshall B. Long, Mitchell D. Smooke</i>	

SESSION B-3 : LAMINAR FLAMES

B-16 Laminar Flame Speeds of Cyclohexane and Mono-alkylated Cyclohexanes at Elevated Pressures	331
<i>Fujia Wu, Andrew Kelley, Chung K. Law</i>	
B-17 NTC-affected Ignition in Nonpremixed Counterflow	349
<i>Chung K. Law, Peng Zhao</i>	
B-18 Prediction of Electron and Ion Concentrations in Low Pressure Premixed Acetylene and Ethylene Flames	374
<i>John Cancian, Beth Anne V. Bennett, Meredith B. Colket, Mitchell D. Smooke</i>	
B-19 Laminar Burning Speed of 1,1-difluoroethane (R152a)/Air Mixtures	378
<i>Casey Bennett, Ali Moghaddas, Hameed Metghalchi</i>	
B-20 Laminar Flame Speeds of Hydrofluorocarbon-Air Mixtures	385
<i>Paul Papas, Shiling Zhang, S. P. Zeppieri, M. B. Colket, K. Smith, Susnane M. Opalka, Parmesh Verma</i>	
B-21 Computational and Experimental Study of Laminar Coflow Methane-air Diffusion Flames Under Elevated Pressures	392
<i>Su Cao, Beth Anne V. Bennett, Bin Ma, Marshall B. Long, Mitchell D. Smooke</i>	
B-22 Sustained Methane/Air Combustion by Pulsed Microwave Energy Deposition	396
<i>James B. Michael, Richard B. Miles</i>	

SESSION B-4: LAMINAR FLAMES

B-23 Direct Ignition and the S-curve Transition by In-situ Nano-second Pulsed Discharge in Methane/Oxygen/Helium Counterflow Flame	405
<i>Wenting Sun, Sang Hee Won, Yiguang Ju</i>	
B-24 An Implicit-compact Finite Difference Method with Application to Forced and Unforced Oscillating Laminar Jet Diffusion Flames	414
<i>Richard Dobbins, Mitchell D. Smooke</i>	
B-25 Computational and Experimental Study of an Axisymmetric Laminar Coflow N-heptane Flame	419
<i>Beth Anne V. Bennett, Charles S. McEnally, Lisa D. Pfefferle, Mitchell D. Smooke</i>	
B-26 Effects of Variable Specific Heats on Markstein Lengths and Flame Front Stability	424
<i>Fujia Wu, John K. Bechtold, Chung K. Law</i>	
B-27 On Self-Acceleration of Cellular Spherical Flames	432
<i>Fujia Wu, Grunde Jomaas, Chung K. Law</i>	
B-28 A Comprehensive Evaluation of Soret Diffusion in Heptane-Air Flames	451
<i>Yuxuan X. Xin, Chih-Jen Sung, Chung K. Law</i>	

SESSION B-5: SPRAYS, DROPLETS & DIAGNOSTICS

B-29 Methanol Droplet Extinction in Oxygen/Carbon-dioxide/Nitrogen Mixtures in Microgravity: Results from the International Space Station Experiments	464
<i>Vedha Nayagam, Daniel Dietrich, Paul Ferkul, Michael Hicks, Forman Williams</i>	
B-30 Flash Atomization of a Superheated Jet Fuel	470
<i>Jeremiah Lee, May Corn, W. Zhao, C. Fotache, S. Gopalakrishnan, David Schmidt</i>	
B-31 Comparison of the Spherically Symmetric Droplet Burning Characteristics of Jet-A with Three and Four Component Surrogate Blends	476
<i>Yu-Cheng Liu, Anthony J. Savas, C. Thomas Avedisian</i>	
B-32 On the Extinction Characteristics of Alcohol Droplet Combustion Under Microgravity Conditions - A Numerical Study	481
<i>Tanvir Farouk, Frederick L. Dryer</i>	
B-33 A Film Boiling Reactor for Decomposition of Subcooled Organic Liquids	491
<i>Wei-Chih Kuo, C. Thomas Avedisian, Wing Tsang</i>	
B-34 Absolute Light Calibration in Combustion Experiments	496
<i>Bin Ma, Marshall Long</i>	
B-35 Selective Observation of the Anomalous Zeeman Effect Using Magneto-optic Rotation	503
<i>Jamie Lane, Michael Stichter, Nicholas Cernansky, David Miller</i>	
B-36 H₂O Number Density and Temperature Measurements in a Rapid Compression Machine Using Mid-IR Absorption Spectroscopy	510
<i>Mruthunjaya Uddi, Apurba K. Das, Goutham Kukkadapu, Chih-Jen Sung</i>	

C-1: TURBULENT FLAMES

C-01 Calculations of a Bluff-body-stabilized Non-premixed Flame Using a Reduced Description with Tabulation of Chemistry	514
<i>Zhuyin Ren, Graham M. Goldin, Varun Hiremath, Stephen B. Pope</i>	
C-02 Turbulence-chemistry Closure Method Using Graphics Processing Units: A Preliminary Test	525
<i>Kyle E. Niemeyer, Chih-Jen Sung, Catalin G. Fotache, Jeremiah Lee</i>	
C-03 Large Eddy Simulation of Turbulence and Surface Catalysis Interaction in a Variable Pressure Flow Reactor	530
<i>Tanvir Farouk, Stephen Dooley, Frederick L. Dryer</i>	
C-04 Large Eddy Simulation of Local Entropy Generation in a Turbulent Mixing Layer	537
<i>M. R. H. Sheikhi, M. Safari, H. Metghalchi</i>	
C-05 Direct Numerical Simulation of Soot Formation and Oxidation in Temporally Evolving Turbulent Luminous Non-Premixed Flames	542
<i>P. G. Arias, V. R. Lecoustre, S. Roy, W. Wang, Z. Luo, D. C. Haworth, H. G. Im, T. F. Lu, K. L. Ma, R. Sankaran, A. Trouvé</i>	
C-06 A Computational Study on the Influence of Exhaust Gas Recirculation on NO_x Emissions for a Swirl Combustor Using Steady and Time Dependent RANS Simulations	556
<i>Sergio Escobar, Jose Escobar, Ismail Celik</i>	
C-07 Auto-ignition and Low Temperature Combustion in HCCI for Nonhomogeneous DME/Air Mixtures	564
<i>Hossam A. El-Asrag, Yiguang Ju</i>	

SESSION C-2: TURBULENT FLAMES

C-08 PDF-based Simulations of Turbulent Spray Combustion in a Constant-Volume Chamber	578
<i>Subhasish Bhattacharjee, Jaishree Jaishree, Vivek Raj Mohan, Hedan Zhang, Daniel C. Haworth</i>	
C-09 LES/PDF Studies of Turbulent Premixed Jet Flames	583
<i>Haifeng Wang, Stephen B. Pope</i>	
C-10 Transported PDF Modeling of Nonpremixed Turbulent Syngas Flames and 0.8 MW Oxy-Natural Gas Furnace	591
<i>Xinyu Zhao, Daniel C. Haworth, E. David Huckaby</i>	
C-11 Blowoff Dynamics of Acoustically Coupled Bluff Body Stabilized Flames Using Proper Orthogonal Decomposition	596
<i>Kristin Kopp-Vaughan, Trevor R. Jensen, John J. Turner, Baki M. Cetegen, Michael W. Renfro</i>	
C-12 Blowoff Scaling of Bluff Body Stabilized Flames	606
<i>C. W. Foley, J. Seitzman, T. Liewen</i>	

C-13 Phase-resolved Characterization of Conical Premixed Flames Near and Far from Blowoff	615
<i>Sayan Biswas, Kristin M. Kopp-Vaughan, John Turner, Michael W. Renfro, Baki M. Cetegen</i>	
C-14 Analysis of Intrinsic Flamefront Instabilities in Response to External Acoustic Forcing	616
<i>V'Yacheslav B. Akkerman, Chung K. Law</i>	
C-15 Darrieus-Landau and Rayleigh-Taylor Instabilities in Outwardly-propagating, Accelerating Flames	625
<i>V'Yacheslav B. Akkerman, Chung K. Law</i>	

SESSION C-3: TURBULENT FLAMES AND STATIONARY COMBUSTION

C-16 Effect of Coal Particles on the Turbulent Burning Velocity of Methane-Air Premixed Flames	632
<i>Scott Rockwell, Ali S. Rangwala</i>	
C-17 Temperature of Inverse Diffusion Flames in a Vitiated Cross-flow Using Two-color PLIF Thermometry	637
<i>Stanislav Kostka, David Blunck, Naibo Jiang, Amy Lynch, Marc Polanka, Scott Stouffer, James R. Gord, Sukesh Roy</i>	
C-18 Turbulent Flame Speed and Self-similar Propagation of Expanding Premixed Flames	648
<i>Swetaprovo Chaudhuri, Fujia Wu, Delin Zhu, Chung K. Law</i>	
C-19 Use of Exhaust Gas Recirculation As a Control Approach for Thermoacoustic Instabilities	659
<i>Joseph Ranalli, D. Ferguson</i>	
C-20 An Experimental Study on Hydrocarbon Emissions in Glycerol Combustion Utilizing GC/TCD/FID	665
<i>Myles D. Bohon, William L. Roberts</i>	
C-21 Pressurized Glycerin Combustion in a Gas Turbine GPU	670
<i>Joseph A. Scroggins, Brian J. McCann, Myles D. Bohon, Joel C. Lisanti, Prithwish Kundu, William L. Roberts</i>	
C-22 Acrolein and Other Volatile Organic Emissions from the Combustion of Crude Glycerol	676
<i>Scott A. Steinmetz, Jason S. Herrington, Chris Winterrowd, Daniel Janek, William L. Roberts, Jost O. L. Wendt, William P. Linak</i>	

SESSION C-4: HETEROGENEOUS COMBUSTION

C-23 Differences of Single-coal Particle Ignition Mechanisms in N₂ and CO₂-Rich Environments	682
<i>Reza Khatami, Yiannis A. Levendis</i>	
C-24 Gaseous and Particulate Emissions from Conventional Combustion and Oxy-combustion of a Lignite Coal	692
<i>Feyza Kazanc, Yiannis Levendis</i>	
C-25 Catalytic Ignition and Heat Release of Ethylene/Air Mixtures Over Palladium Oxide	700
<i>Yuxuan Xin, Chung K. Law</i>	
C-26 Multiphysics Modeling of Coal Gasification Processes in a Well-stirred Reactor with Detailed Gas-phase Chemistry	708
<i>Li Qiao, Jian Xu, Jay Gore</i>	
C-27 Combustion of Nanofluid Fuels with the Addition of Boron and Iron Particles at Dilute and Dense Concentrations	722
<i>Yanan Gan, Yi Syuen Lim, Li Qiao</i>	
C-28 Enhanced Evaporation of Nanofluids by Radiation Absorption of Nanoparticles	743
<i>Yanan Gan, Li Qiao</i>	

SESSION C-5: FIRE

C-29 Study of Interaction of Entrained Coal Dust Particles in Lean Methane-Air Premixed Flames	756
<i>Yanxuan Xie, Vasudevan Raghavan, Ali S. Rangwala</i>	
C-30 Numerical Modeling of Spontaneous Ignition of Coal Dust Layers Deposited Over Hot Surfaces	765
<i>Kulbhushan A. Joshi, Ali S. Rangwala, V. Raghavan</i>	
C-31 Catalytic Ignition of Enclosed Hydrogen Leaks	771
<i>Kyle Brady, Chih-Jen Sung, James S. T'ien</i>	
C-32 Piloted Ignition Regimes of Wildland Fuel Beds	775
<i>J. C. Thomas, Albert Simeoni, Francesco Colella, Jose L. Torero</i>	
C-33 Stirred-Reactor Simulations of Enhanced Reaction in the Presence of Fire Suppressants	780
<i>G. T. Linteris, D. R. Burgess, F. Takahashi, V. R. Katta, O. Meier</i>	

C-34 Dynamics of Interactions of a Watermist Spray with a Buoyant Plume	785
<i>Ragini Acharya, Guido Poncia</i>	
C-35 Conditions Affecting External Flame Propagation Into a Portable Gasoline Container: A Summary of Test Methods and Experimental Findings	793
<i>Brian E. Elias, Robert G. Zalosh, Ali S. Rangwala</i>	
Author Index	