

**2007 FALL TECHNICAL MEETING
EASTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE
University of Virginia
Monday, October 22, 2007**

8:00 **Registration**
8:15 **Welcome Remarks: James Aylor, Dean, School of Engineering, University of Virginia**
8:30 **Invited Speaker: Session Chair:**
 Modeling wildland and wildland-urban interface fires.
 William “Ruddy” Mell, National Institute of Standards & Technology
Announcements – Harsha Chelliah, University of Virginia

	A-1: Reaction Kinetics I (room 1) Session Chair: Prof. Joseph Bozzelli	B-1: New Technology (room-2) Session Chair: Prof. Jerry Seitzman	C-1: Fire Research (room-3) Session Chair: Dr. Charles McEnally
9:30	A-01 Theoretical study of the combustion and thermal decomposition of RDX Part I: Kinetic modeling. <i>William R. Anderson², Gabriel da Silva¹, Joseph W. Bozzelli¹, Clint B. Conner²</i> ¹ <i>New Jersey Institute of Technology,</i> ² <i>US Army Research Laboratory</i>	B-01 Experimental investigation of kinetic ignition of counterflow diffusion flames by plasma-activated ultra-lean premixtures. <i>Timothy Ombrello, Yiguang Ju,</i> <i>Princeton University</i>	C-01 Evolved combustion products from CNT-polymer composites. <i>Randy L. Vander Wal¹, Jane Fujiyama-Novak¹, Vladimir Pushkarev²,</i> ¹ <i>The NCSE at The NASA-Glenn Research Center;</i> ² <i>Carnegie Mellon University</i>
9:50	A-02 Theoretical study of the combustion and thermal decomposition of RDX Part II: Detailed kinetics on initial reaction paths. <i>Gabriel da Silva, Joseph W. Bozzelli,</i> <i>New Jersey Institute of Technology</i> <i>Clint B. Conner, William R. Anderson,</i> <i>US Army Research Laboratory</i>	B-02 Modeling of carbon nanotube growth by flame synthesis. <i>Sayangdev Naha, Ishwar K. Puri,</i> <i>Virginia Polytechnic Institute and State University</i>	C-02 Numerical modeling of two-dimensional smolder structure. <i>Amanda Dodd, Chris Lautenberger,</i> <i>Carlos Fernandez-Pello,</i> <i>University of California, Berkeley</i>
10:10	BREAK		

10:30	A-03 Chemically activated oxidation of n-propyl radicals. <i>Wing Tsang</i> <i>National Institute of Standards and Technology</i>	B-03 Electrostatic self-assembly of a nanoscale thermite system into ordered microspheres. <i>Jonathan Y. Malchi, Richard A. Yetter, Pennsylvania State University,</i> <i>Timothy J. Foley, Los Alamos National Lab</i>	C-03 Three-dimensional simulation of suppression of flames by water-mist injection. <i>Douglas Schwer, K Kailasanath,</i> <i>Naval Research Laboratory</i>
10:50	A-04 Ab initio chemical kinetics for N₂ reaction with singlet and triplet CH₂ radicals. <i>Shucheng Xu, M.C. Lin, Emory University</i>	B-04 Development and preliminary testing of an electrolytic ignition microthruster for space propulsion. <i>Ming-Hsun Wu, National Cheng Kung University;</i> <i>Richard A. Yetter, Pennsylvania State University</i>	C-04 Experimental comparison of opposed and concurrent flame spread in a forced convective microgravity environment. <i>S.L. Olson, F.J. Miller</i> <i>NASA Glenn Research Center at Lewis Field</i>
11:10	A-05 New shock-tube facility for studies in chemical kinetics at engine conditions. <i>C.J. Aul, J. de Vries, E.L. Petersen</i> <i>University of Central Florida</i>	B-05 A chemical process for converting lipids to transportation fuels. <i>T.L. Turner, Permafuels, Inc.,</i> <i>W.L. Roberts, L.F. Stikeleather, NC State Univ.</i>	C-05 Limiting length and non-growing flames in concurrent flow over thick solids. <i>Ya-Ting Tseng, James S. T'ien,</i> <i>Case Western Reserve University</i>
11:30	A-06 Preignition oxidation chemistry of n-decane. <i>Matthew S. Kurman, Robert H. Natelson,</i> <i>Nicholas P. Cernansky, David L. Miller</i> <i>Drexel University</i>	B-06 A study of emissions from diesel and vegetable oil fueled vehicles. <i>Timothy A. Bockus, John D. Mertens,</i> <i>Trinity College</i>	C-06 Promotion of hydrogen-air ignition by iron compounds. <i>Gregory Linteris,</i> <i>National Institute of Standards and Technology</i>
11:50	A-07 Molecular dynamics study of C-C bond dissociation in linear alkanes and polyethylene: effects of condensed phase. <i>Konstantin V. Popov, Vadim D. Knyazev</i> <i>Catholic University of America</i>	B-07 Study of reaction rates through a local extinction point in non-premixed flames. <i>William F. Carnell, Jr., Milwaukee School of Engineering;</i> <i>Michael W. Renfro,</i> <i>University of Connecticut</i>	C-07 Radiative pyrolysis of JA2 from an electrochemical plasma discharge. <i>Malay K. Das, Arindrajit Chowdhury,</i> <i>Stefan T. Thynell, Pennsylvania State University</i>
12:30	LUNCH		
1:30	Invited Speaker II: Session Chair: <i>Modeling and simulation of solid energetic material combustion and ignition. Vigor Yang, Pennsylvania State University</i>		

	Session A-2: Internal Combustion Engines (room - 1) Session Chair: Prof. Tiegang Fang	Session B-2: Laminar Flames I (room - 2) Session Chair: Prof. Yiguang Ju	Session C-2: Soot (room - 3) Session Chair: Prof. Beei-Huan Chao
2:30	A-08 Investigation of scaling issues in small internal combustion engines. <i>Shyam Menon, Christopher Cadou, University of Maryland at College Park</i>	B-08 A simple model for a small wick flame. <i>Howard R. Baum, University of Maryland and National Institute of Standards and Technology</i>	C-08 Sooting tendencies of nonvolatile aromatic hydrocarbons. <i>Charles S. McEnally, Lisa D. Pfefferle, Yale University</i>
2:50	A-09 Methane and dimethyl ether oxidation at elevated temperatures and pressures. <i>Christopher Zinner, Eric Petersen, University of Central Florida</i>	B-09 Computational and experimental study of oxygen-enhanced axisymmetric laminar methane flames. <i>Beth Anne V. Bennett¹, Zhongxian Cheng², Robert W. Pitz²; Mitchell D. Smooke¹, ¹Yale University; ²Vanderbilt University</i>	C-09 Laminar smoke points of waxes. <i>K.M. Allan, J.R. Kaminski, J.C. Bertrand, J. Head, P.B. Sunderland, University of Maryland at College Park</i>
3:10	BREAK		
3:30	A-10 Rate-controlled constrained-equilibrium calculations of the combustion products in the expansion stroke of an internal combustion engine. <i>M. Janbozorgi, D. Goldthwaite, H. Metghalchi, Northeastern University; C. Keck, Massachusetts Institute of Technology</i>	B-10 Effects of ethylene addition on conterflow ignition and flame propagation in methane/ethylene mixtures. <i>W. Liu¹, Y. Huang², T.F. Lu, D.L. Zhu, C.K. Law¹ ¹Princeton University, ²University of Iowa</i>	C-10 The impact of detailed multicomponent transport and thermal diffusion effects on soot formation in ethylene/air flames. <i>Seth B. Dworkin, Mitchell D. Smooke, Yale University, Vincent Giovangigli, Ecole Polytechnique</i>
3:50	A-11 Transported PDF modeling for a direct-injection PCCI engine. <i>Eugene H. Kung, Daniel C. Haworth, Pennsylvania State University</i>	B-11 Nonlinear effects in the experimental determination of laminar flame properties from stretched flames. <i>Andrew P. Kelley, Chung K. Law, Princeton University</i>	C-11 Modeling the effect of flame structure on the formation of aromatics in opposed flow diffusion flames. <i>Scott A. Skeen, Richard L. Axelbaum, Washington University in Saint Louis</i>

4:10	A-12 Computational fluid dynamics study of combustion in a rapid compression machine. <i>Gaurav Mittal, Mandhpati P. Raju, Chih-Jen Sung, Case Western Reserve University</i>	B-12 Structure of fuel/oxygen/diluent (argon, helium, nitrogen) premixed flames at high pressures and temperatures. <i>Kian Eisazadeh Far, Raymond J. Andrews, Hameed Metghalchi, Northeastern University; Farzan Parsinejad, Chevron Corporation</i>	C-12 Effects of C/O ratio and scalar dissipation rate on sooting limits of spherical non-premixed flames. <i>V.R. Lecoustre¹, B.H. Chao², P.B. Sunderland¹, D.L. Urban³, D.P. Stocker³, Richard Axelbaum⁴; ¹University of Maryland, ²University of Hawaii; ³NASA Glenn ⁴Washington University in St Louis</i>
4:30	A-13 A rapid compression machine study of dimethyl ether autoignition. <i>Gaurav Mittal¹, Marcos Chaos², Chih-Jen Sung¹, Frederick L. Dryer², ¹Case Western Reserve University, ²Princeton University</i>	B-13 The structure of a JP-8 counterflow diffusion flame by gas sampling and GC/MS analysis. <i>L. Tosatto, B. La Mantia, P. Duchaine, M.D. Smooke, A. Gomez, Yale University</i>	C-13 Evidence for polynuclear aromatic hydrocarbon aggregation in flames: Intermolecular potential calculations. <i>Jennifer D. Herdman, J. Houston Miller, George Washington University</i>
5:00 6:30	GENERAL BUSINESS MEETING BANQUET remarks from Professor John Fenn		
8:30	Tuesday, October 23, 2007 Invited Speaker III: Session Chair: <i>Supersonic combustion research at NASALaRC.</i> Philip Drummond, NASA Langley Research Center		
	Session A-3: Reaction Kinetics II (room – 1) Session Chair: Dr. Iftikhar Awan	Session B-3 : Turbulent Flames (room – 2) Session Chair: Prof. Michael Renfro	Session C-3: Heterogeneous Combustion (room – 3) Session Chair: Dr. Giuliano Amantini
9:30	A-14 Shock-tube study of the ignition delay times of ethanol at high pressures and intermediates temperatures experimental and numerical approaches. <i>M. Fikri¹, L.R. Cancino², A A. Oliveira², C. Schulz¹; ¹Universität Duisburg-Essen, Germany, ²Federal University of Santa Catarina- Brazil</i>	B-14 Soot Topography in a Planar Diffusion Flame Wrapped by Interacting Line Vortices. <i>S. Basu, University of Central Florida, S. Chaudhuri, B.M. Cetegen University of Connecticut</i>	C-14 Size resolved kinetics of nickel nanoparticle oxidation by ion-mobility classification. <i>Lei Zhou, Ashish Rai, Nicholas Piekiet, Xiaofei Ma, Michael R. Zachariah, University of Maryland</i>

9:50	<p>A-15 The kinetics and mechanism for the unimolecular decomposition of acetophenone: <i>Ab Initio</i> MO and VTST/RRKM calculations. S.P. Ju¹, H.T. Chen², M.C. Lin²⁻³, J.G. Chang⁴, M.H. Weng¹; ¹National Sun-Yat-Sen University, ²National Chiao Tung University, ³Emory University, ⁴National Center for High-Performance Computing</p>	<p>B-15 Assessment of RANS-based turbulent combustion models for prediction of gas turbine emissions: turbulence model and reaction mechanism effects. Jagannath Nanduri, Ismail Celik, Don Parsons, West Virginia University, Peter Strakey, National Energy Technology Laboratory</p>	<p>C-15 High pressure shock tube studies on C(s)+CO₂. Brad Culbertson, Raghu Sivaramakrishnan, Kenneth Brezinsky, University of Illinois at Chicago</p>
<p>10:10</p> <p>BREAK</p>			
10:30	<p>A-16 Measurements of HCN and C₂H₂ from a pyridine-doped methane/air axisymmetric flame using cavity ringdown spectroscopy. Eric Fallows, Maria Puccio, J. Houston Miller George Washington University</p>	<p>B-16 Instantaneous flamelet displacement speed measurements on a premixed turbulent V-flame. S.S. Sattler, TIAX, LLC F.C. Gouldin, Cornell University</p>	<p>C-16 On the modeling of porous carbon particle combustion. J.L. Kassebaum, H.K. Chelliah University of Virginia</p>
10:50	<p>A-17 Chain branching and termination paths in oxidation of <i>n</i>-alkanes: Comprehensive complete basis set-QB3 study on the association of <i>n</i>-pentyl radical with O₂, Isomerization and addition of second oxygen molecule. Rubik Asatryan, Joseph W. Bozzelli, New Jersey Institute of Technology</p>	<p>B-17 PDF modeling of turbulent lean premixed combustion. Server Levent Yilmaz, Peyman Givi, University of Pittsburgh Peter A. Strakey, National Energy and Technology Laboratory</p>	<p>C-17 Influences of temperature and available carbon sources on synthesis of carbon nanotubes in methane-air diffusion flames. Tianxiang Li, Kozo Saito, Hongguo Zhang, Zhi Chen, University of Kentucky Kazunori Kuwana, University of Tokyo</p>
11:10	<p>A-18 The high pressure combustion of saturated and unsaturated C₇ hydrocarbons. Stephen W. Garner, Raghu Sivaramakrishnan, Kenneth Brezinsky, University of Illinois at Chicago; Philippe Dagaut, CNRS, France</p>	<p>B-18 Effects of spatial mixture gradients on stabilization zone temperatures of bluff-body stabilized turbulent premixed conical flames. S. Chaudhuri, B.M. Cetegen, University of Connecticut</p>	<p>C-18 Deflagrations of nitromethane and nanoaluminum mixtures. Justin Sabourin, Richard Yetter, Grant Risha, Pennsylvania State University; Blaine Asay, Los Alamos National Laboratory; Steven Son, Purdue University</p>

11:30	A-19 Thermochemistry and kinetics of the alpha-hydroxyethyl radical + O₂ reaction in ethanol combustion. <i>Gabriel da Silva, Long Liang, Joseph W. Bozzelli, New Jersey Institute of Technology, John Farrell, ExxonMobil Research & Engineering Co.</i>	B-19 Temperature measurements in the stabilization zone of acoustically modulated, turbulent premixed conical flames by emission spectroscopy. <i>S. Chaudhuri, B.M. Cetegen, University of Connecticut</i>	C-19 Dependence of the combustion velocity on particle size and pressure for an Al/CuO thermite. <i>Michael Weismiller, J.Y. Malchi, R.A. Yetter, Pennsylvania State University; Tim Foley, Los Alamos National Laboratorie</i>
11:50	A-20 Flow reactor pyrolysis of diethyl sulfide. <i>Xin Zheng, E.M. Fisher, F.C. Gouldin, Cornell University; Li Zhu, J.W. Bozzelli, New Jersey Institute of Technology Newark</i>	B-20 Radiation-driven flame weakening effects in sooting turbulent diffusion flames. <i>P. Narayanan, A. Trouvé, University of Maryland</i>	C-20 Effects of dioctyl sulfosuccinate on the burning rate of HTPB/AP solid composite propellants. <i>M.A. Stephens, D. Reid, G. Carro, A. LePage, S. Seal, E.L. Petersen University of Central Florida</i>
12:15	LUNCH		
1:30	Invited Speaker IV: Session Chair: <i>Computational and experimental study of soot formation in coflow diffusion flames. Mitchell D. Smooke, Yale University</i>		
	Session A-4: Sprays and IC Engines (room – 1) Session Chair: Prof. Peter Sunderland	Session B-4: Unsteady Combustion (room – 2) Session Chair: Dr. Gregory Linteris	Session C-4: Catalytic Combustion (room – 3) Session Chair: Dr. Eric Petersen
2:30	A-21 Combustion in an optical Diesel engine fueled with Diesel and bio-diesel fuels using multiple injection strategies. <i>Tiegang Fang, North Caroline State University, Chia-Fon F. Lee, University of Illinois at Urbana-Champaign</i>	B-21 Response of premixed flames to equivalence ratio oscillations: Non-quasi steady effects. <i>Shreekrishna, Tim Lieuwen, Georgia Institute of Technology</i>	C-21 A first-principles study on the sublimation/decomposition of NH₄ClO₄. <i>R.S. Zhu, M.C. Lin, Emory University</i>

2:50	A-22 High efficiency residual oil (SuperHERO) gun for liquid waste incineration. <i>I-Ping Chung and Joe Colannino, John Zink Company</i>	B-22 Auto-ignition of homogeneous hydrogen/air mixture subjected to unsteady temperature fluctuations. <i>Gaurav Bansal, Hong G. Im, University of Michigan; Su-Ryong Lee, Seoul National University of Technology</i>	C-22 Single-walled Carbon Nanotube Growth from Composite Catalysts in Diffusion Flames. <i>Chad J. Unrau, Richard L. Axelbaum, Washington University in St Louis</i>
3:10	BREAK Women in Combustion Coffee		
3:30	A-23 Intensity and efficiency of polydispersed spray fuel-fed well-mixed combustors. <i>Daniel E. Rosner, Manuel Arias-Zugasti, Michael Labowsky, Yale University</i>	B-23 Predicting dynamic heat release rate in turbulent flames with reduced-order models. <i>Christopher Martin, Joe Ranalli, Paul Black, William Baumann, Uri Vandsburger, Robert West, Virginia Polytechnic Institute and State University</i>	C-23 Effects of heat loss on a stagnation-point flow catalytic combustor. <i>Jingjing Li, Hong G. Im, James Wiswall, Margaret S. Wooldridge, University of Michigan</i>
3:50	A-24 A new detailed numerical model of isolated droplet combustion. <i>Kenneth Kroenlein, Andrei Kazakov, Frederick L. Dryer, Princeton University</i>	B-24 Numerical investigation of acoustic wave interaction with 2-D counter flow flames. <i>A.T. Sriram, H.K. Chelliah, University of Virginia</i>	C-24 Upstream flame propagation in catalytic microtubes. <i>Michael Johnston, National Center for Space Exploration Research; Fletcher Miller, San Diego State University; Daniel Dietrich, Peter Struk,, NASA Glenn Research Center; James T'ien, Case Western Reserve University</i>
4:10	A-25 Confined rapid thermolysis/FTIR spectroscopy/ToF mass spectrometry of TAGzT. <i>Arindrajit Chowdhury, Stefan T. Thynell, Pennsylvania State University</i>	B-25 Fuel interchangeability consideration for gas turbine combustion. <i>Don Ferguson, National Energy Technology Laboratory-US DOE</i>	C-25 Role of the Knudsen layer in determining surface reaction rates based on sticking coefficients. <i>Peng Zhang, Chung K. Law, Princeton University</i>
Wednesday, October 24, 2007			
8:30	Invited Speaker V: Session Chair: <i>Recent advances in propulsion at GE.</i> Keith McManus, GE Research		
	Session A-5: Reaction Kinetics III (room – 1) Dr. Tianfeng Lu	Session B-5: Laminar Flames II (room – 2) Dr. Beth Anne Bennett	Session C-5: Turbulent Flames II (room – 3) Session Chair: Prof. Arnaud Trouvé

9:30	A-26 Optimization of combustion application codes using sparse matrix techniques. <i>Mandhapati P. Raju, Chih Jen Sung, Case Western Reserve University</i>	B-26 The stretch effect on the accurate determination of laminar flame speed using expanding flames in a spherical bomb. <i>Zheng Chen, Yiguang Ju, Princeton University</i>	C-26 Turbulent combustion velocimetry in a scramjet. <i>Chad Smith, Chris Goyne, University of Virginia</i>
9:50	A-27 Integrating sensitivity analysis into directed relation graph with error propagation for effective mechanism reduction. <i>Mandhapati P. Raju, Chih Jen Sung, K.P. Kundu, Case Western Reserve University</i>	B-27 Calculated extinction strain rates for binary fuel mixtures. <i>Okjoo Park, Elizabeth M. Fisher, Cornell University</i>	C-27 Effects of coaxial air on nitrogen-diluted hydrogen jet diffusion flame length and NO_x emission. <i>Nathan Weiland¹, Ruey-Hung Chen², Peter Strakey¹; ¹ National Energy Technology Laboratory, ² University of Central Florida</i>
10:10	BREAK		
10:30	A-28 Error control of model reduction by linearized quasi steady state approximation. <i>Xiaoxia Dong, William H. Green, Massachusetts Institute of Technology</i>	B-28 Laminar flame speeds of H₂/CO/O₂/He mixtures at elevated pressure and preheat temperature. <i>Jayaprakash Natarajan, Yash Kochar, Tim Lieuwen, Jerry Seitzman, Georgia Institute of Technology</i>	C-28 Simultaneous 2-line OH Thermometry and PIV of unsteady methane-air kernel-vortex interactions. <i>Sean Danby, William Roberts, North Carolina State University</i>
10:50	A-29 <i>Ab initio</i> chemical kinetics and mechanism for the CH₃O + O (3P) reaction. <i>Z.F. Xu, M.C. Lin, Emory University</i>	B-29 Quenching limits of hydrogen diffusion flames. <i>Michael Butler, Richard Axelbaum, Washington University in Saint Louis; Chris Moran, Peter Sunderland, University of Maryland</i>	C-29 Effects of the leading-edge reaction zone on lifted flame oscillations. <i>N.J. Moore, K.M. Lyons, North Carolina State University</i>
11:10	A-30 Kinetic modeling of the benzyl + HO₂ reaction. <i>Gabriel da Silva, Joseph W. Bozzelli, New Jersey Institute of Technology</i>	B-30 A paradigm shift in the interaction of experiments and computations in combustion research. <i>Blair C. Connelly, Beth Anne V. Bennett, Mitchell D. Smooke, Marshall B. Long, Yale University</i>	C-30 Composition PDF/method of moments modeling of soot formation in a turbulent ethylene/air jet flame. <i>Ranjan S. Mehta, Daniel C. Haworth, Michael F. Modest, Pennsylvania State University</i>

<p>11:30</p>	<p>A-31 Sensitivity analysis for the thermal gas phase reactions of 5-methyl-hexyl radicals. <i>Iftikhar A. Awan, Wing Tsang, W. Sean McGivern, Jeffrey A. Manion National Institute of Standards and Technology</i></p>	<p>B-31 Stretch effects on the stability of spherical premixed flames. <i>Grunde Jomaas, Chung K. Law, Princeton University</i></p>	<p>C-31 Three-dimensional numerical simulation of flames supported by a spinning porous-plug burner. <i>K.N. Hossain, T.L. Jackson, J. Buckmaster Buckmaster Research</i></p>
<p>11:50</p>			<p>C-32 Effect of cylindrical confinement on the evolution of outwardly propagating flames. <i>M.P. Burke, Y. Ju, F.L. Dryer; Princeton University</i></p>