

Fall Technical Meeting of the Eastern States Section of the Combustion Institute 2013

**Clemson, South Carolina, USA
13 - 16 October 2013**

ISBN: 978-1-62993-719-9

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**2013 FALL TECHNICAL MEETING
EASTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE
Clemson University, South Carolina
October 13-16, 2013**

Sunday, October 13, 2013

6:00 – 8:00 Madren Center Connector and Patio: Registration and Reception

Monday, October 14, 2013

7:30 Madren Center Connector: Registration
8:15 Bell South Auditorium: Welcome Remarks/Announcements: W.L. Roberts, KAUST, ESSCI Chair

8:30 Session Chair: W.L. Roberts
Invited Speaker: Daniel C. Haworth, Pennsylvania State University
Title: *Toward predictive CFD models for advanced compression-ignition engines: Accounting for unresolved turbulent fluctuations*

	A-1: Turbulent Flames Bell South Auditorium Session Chair: B.M. Cetegen	B-1: Diagnostics Ballroom C Session Chair: M.J. Gollner	C-1: Soot Seminar Room II Session Chair: P.B. Sunderland
9:40	A-01 Subgrid-scale mixing of temperature perturbations from flamelet in turbulent partially premixed flames"³" <i>S. Liu, C. Tong Clemson University</i>	B-01 Formaldehyde fluorescence as a marker for scalar dissipation through local extinction <i>Kathryn R. Gosselin, William F. Carnell, Jr.,³89 Michael W. Renfro University of Connecticut</i>	C-01 Soot measurements in high-pressure laminar diffusion flames"⁵³: <i>S.A. Steinmetz¹, T. Fang², W.L. Roberts^{1,2} ¹KAUST ²North Carolina State University</i>
10:00	A-02 Chemiluminescence imaging of a reacting jet in a vitiated crossflow"⁹ <i>Jason A. Wagner, George M. Lapaan, Michael W. Renfro, Baki M. Cetegen University of Connecticut</i>	B-02 Development of a LED-based sensor for simultaneous, time-resolved measurements of CO and CO₂ from combustion exhausts"³⁹⁵ <i>Kyle Thurmond¹, Emmanuel Duenas¹, Subith S. Vasu¹, William P. Partridge, Jr.² ¹University of Central Florida ²Oak Ridge National Laboratory</i>	C-02 Observations of a hydrocarbon-free soot flame"⁵⁴⁶ <i>Paul M. Anderson, Haiqing Guo, Peter B. Sunderland University of Maryland</i>
10:20	BREAK – Corridor		

	A-1: Turbulent Flames (cont.) Session Chair: B.M. Cetegen	B-1: Diagnostics (cont.) Session Chair: M.J. Gollner	C-1: Soot (cont.) Session Chair: P.B. Sunderland
10:50	A-03 Flame leading point stretch statistics of negative Markstein length fuels""37 <i>Andrew Marshall, Prabhakar Venkateswaran, Jerry Seitzman, Tim Lieuwen</i> <i>Georgia Institute of Technology</i>	B-03 Bench-scale apparatus for studying pool fire extinguishment by Class B foams""39; <i>Ramagopal Ananth, Sutton Mott, Majid Waheed, Maximilian Epstein, James M. Smith, Michael W. Conroy, James W. Fleming</i> <i>Naval Research Laboratory</i>	C-03 Soot formation in butanol isomer non-premixed flames""552 <i>Pradeep Singh, Xin Hui, Chih-Jen Sung</i> <i>University of Connecticut</i>
11:10	A-04 Flame surface statistics of expanding turbulent flame""43 <i>Abhishek Saha¹, Swetaprovo Chaudhuri^{1,2}, Chung K. Law¹</i> <i>¹Princeton University ²Indian Institute of Science</i>	B-04 Modeling suppression of a liquid pool flame by aqueous foams""3: 7 <i>Cedrick Ngalande, James W. Fleming, Ramagopal Ananth</i> <i>Naval Research Laboratory</i>	C-04 Soot and aromatic species in non-premixed and partially-premixed laminar co-flow flames""558 <i>Yefu Wang¹, Suresh S. Iyer¹, Venkatesh R. Iyer¹, Milton J. Linevsky¹, Thomas A. Litzinger¹, Robert J. Santoro¹, Viswanath Katta²</i> <i>¹Pennsylvania State University</i> <i>²Innovative Scientific Solutions Inc.</i>
11:30	A-05 An investigation on fuel similarity of turbulent flames for C₄-C₈ n-Alkanes""49 <i>Fujia Wu, Abhishek Saha, Swetaprovo Chaudhuri, Chung K. Law</i> <i>Princeton University</i>	B-05 Oxidizer dilution extinguishment of a turbulent Wolfhard-Parker flame""3: 3 <i>J.P. White¹, E.D. Link¹, T.M. Myers¹, S.R. Vilfayeau¹, A.W. Marshall¹, P.B. Sunderland¹, A.C. Trouvé¹, J.A. Sheffel², M.L. Corn², M.B. Colket²</i> <i>¹University of Maryland</i> <i>²United Technologies Research Center</i>	C-05 Nanostructure evolution of petroleum based JP-8 and synthetic HRJ, FT derived soot from a gas jet turbine engine""564 <i>Chung-Hsuan Huang, Randy L. Vander Wal</i> <i>Pennsylvania State University</i>
11:50	A-06 Blowoff dynamics of a bluff body stabilized turbulent premixed flame in a cylindrical duct subjected to dual tone velocity oscillation""55 <i>Bikram Roychowdhury, Baki M. Cetegen</i> <i>University of Connecticut</i>	B-06 Numerical simulation of under-ventilated compartment fires""3: 9 <i>S. Vilfayeau¹, N. Ren², Y. Wang², A. Trouvé¹</i> <i>¹University of Maryland ²FM Global</i>	C-06 Soot nanostructure evolution evolves from variations in flame temperature and fuel/air equivalence ratio""56; <i>Chung-Hsuan Huang¹, Jeremy P. Cain², Randy L. Vander Wal¹, William M. Roquemore³</i> <i>¹Pennsylvania State University</i> <i>²University of Dayton</i> <i>³Wright-Patterson Air Force Base</i>
12:10	LUNCH – Ballrooms A & B		
	Bell South Auditorium		
	Session Chair: A. Trouvé		
1:30	Invited Speaker: Yi Wang, FM Global Research		
	Title: CFD modeling of industrial fire protection – progress and challenges		

	Session A-2: Laminar Flames Bell South Auditorium Session Chair: B.A.V. Bennett	Session B-2: Fire Ballroom C Session Chair: M.J. Gollner	Session C-2: Heterogeneous Combustion Seminar Room II Session Chair: H.K. Chelliah
2:40	A-07 Experimental and kinetics studies of acetylene flames at elevated pressures""63 <i>Xiaobo Shen^{1,2}, Xueliang Yang¹, Jeffrey Santner¹, Jinhua Sun², Yiguang Ju¹</i> ¹ Princeton University ² University of Science and Technology of China	B-07 Localized heating ahead of flame front in wildland fire spread""425 <i>Sharif E. Jamaludin¹, Madison Donoho¹, Justin D. English², Brittany A. Adam², Nelson K. Akafuah²</i> ¹ Paul Laurence Dunbar High School ² University of Kentucky	C-07 Coupled heterogeneous and homogeneous oxidation of heated carbon surfaces simulated using the OpenFOAM computational package""579 <i>R.F. Johnson, H.K. Chelliah</i> University of Virginia
3:00	A-08 Measurement of laminar burning speeds and investigation of stability of acetylene (C₂H₂)/air flames""69 <i>Emad Rokni, Ali Moghaddas, Omid Askari, Hameed Metghalchi</i> Northeastern University	B-08 Thermal and burning rate characteristics of laminar boundary layer diffusion flames""42; <i>A.V. Singh, M.J. Gollner</i> University of Maryland	C-08 A parametric study of reactive wave propagation in nanoporous silicon energetic composites""585 <i>Venkata Sharat Parimi, Srinivas A. Tadigadapa, Richard A. Yetter</i> Pennsylvania State University
3:20	BREAK – Corridor		
3:50	A-09 Evaluation of thermal radiation effects on apparent propagation rates of high pressure spherical flames""75 <i>J. Santner, F.M. Haas, Y. Ju, F.L. Dryer</i> Princeton University	B-09 Regional-scale simulations of wildland fire spread using ensemble-based data assimilation""438 <i>Mélanie C. Rochoux^{1,2,3}, Charlotte Emery^{1,2,4}, Sophie Ricci^{1,2}, Bénédicte Cuenot¹, Arnaud Trounev⁴</i> ¹ CERFACS ² CNRS ³ Ecole Centrale Paris ⁴ University of Maryland	C-09 An investigation into the mechanism for the vapor-phase cracking of eugenol""58; <i>Elmer B. Ledesma, Jennifer N. Hoang, Valeria Hernandez, Mitchell Nguyen</i> University of St. Thomas
4:10	A-10 On the uncertainty of extrapolation of laminar flame speed and Markstein length from expanding spherical flames.""7; <i>Fujia Wu¹, Wenkai Liang¹, Chung K. Law¹, Zheng Chen²</i> ¹ Princeton University ² Peking University		C-10 An analysis of transient oxidation of magnetite to hematite in chemical looping combustion""596 <i>Tianxiang Li, Fung Liu, Yunging Han, Kunlei Liu, Kozo Saito</i> University of Kentucky
4:45-6:15	Special Seminar Speaker: Paul Aldo Topic: Effective Presentations Skills Bell South Auditorium		
6:30-8:00	Reception Ballrooms A & B		

Tuesday, October 15, 2013

8:00-10:00 Madren Center Connector: Registration
8:15 Announcements: C. Tong
8:30 Session Chair: C. Tong
 Invited Speaker: Keith R. McManus, GE Global Research Center
 Title: *Low-emissions gas turbine combustion: Design trends and challenges*

	Session A-3: Laminar Flames Bell South Auditorium Session Chair: M. Mueller	Session B-3: Reaction Kinetics Ballroom C Session Chair: C.-J. Sung	Session C-3: New Technology/ Internal Combustion Engines Seminar Room II Session Chair: R.S. Miller
	A-11 MC-Smooth: A mass-conserving, smooth vorticity-velocity formulation for multidimensional flows ⁸⁷ S. Cao, B.A.V. Bennett, M.D. Smooke Yale University	B-11 Non-Boltzmann effects in low-temperature fuel oxidation ⁴⁴⁴ M.P. Burke, C.F. Goldsmith, Y. Georgievskii, S.J. Klippenstein Argonne National Laboratory	C-11 Perovskite catalysts enhanced combustion on porous media ^{5: 2} Manuel D. Robayo, Ben Beaman, Billy Hughes, Brittany Delose, Nina Orlovskaya, Ruey-Hung Chen University of Central Florida
10:00	A-12 Local rectangular refinement in three dimensions (LRR3D) with application to unsteady combustion problems ⁹³ B.A.V. Bennett, M.D. Smooke Yale University	B-12 Using reactive molecular dynamics simulations to refine the mechanism of TMEDA combustion ⁴⁴⁹ Craig D. Needham, Phillip R. Westmoreland North Carolina State University	C-12 Development of a porous combustor for the efficient extraction of thermal energy from liquid and gaseous fuels ^{5: 8} Anthony Carmine Terracciano, Subith S. Vasu, Nina Orlovskaya University of Central Florida
10:20	BREAK - Corridor		
10:50	A-13 Numerical modeling of axi-symmetric laminar diffusion flames with soot ⁹⁹ Adhiraj Dasgupta, Daniel C. Haworth Pennsylvania State University	B-13 A decomposition study of isopropanol in a variable pressure flow reactor ⁴⁵² J.S. Heyne, F.L. Dryer Princeton University	C-13 HCCI engine modeling of diisopropyl ketone, a prototypical biofuel ^{5; 4} Ghazal Barari ¹ , Batikan Koroglu ¹ , Subith S. Vasu ¹ , John E. Dec ² , Craig A. Taatjes ² ¹ University of Central Florida ² Sandia National Laboratories
11:10	A-14 Effects of gravity, radiation, and coflow velocity on laminar coflow methane-air diffusion flames ⁵ S. Cao ¹ , B.A.V. Bennett ¹ , B. Ma ¹ , D. Giassi ¹ , D.P. Stocker ² , F. Takahashi ² , M.B. Long ¹ , M.D. Smooke ¹ ¹ Yale University ² NASA Glenn Research Center	B-14 A comparative study of methane-air and syn gas premixed flames for NO_x formation Atul Joshi, Rajesh Gupta M.A.N.I.T. 458	C-14 Kinetics of NO_x formation from N₂/O₂/C₂H₄/Ar mixtures in repetitively-pulsed dielectric-barrier discharges ^{5; :} Kuminori Togai, Nicholas Tsolas, Richard A. Yetter Pennsylvania State University

	Session A-3: Laminar Flames (cont.) Session Chair: M. Mueller	Session B-3 : Reaction Kinetics (cont.) Session Chair: C.-J. Sung	Session C-3: New Technology/ Internal Combustion Engines Session Chair: R.S. Miller
11:30	A-15 Experimental and computational temperatures in coflow nonpremixed flames <i>C.S. McEnally, B.A.V. Bennett, L.D. Pfefferle, M.D. Smooke</i> Yale University	B-15 A kinetic model for the high-temperature oxidation of <i>n</i>-butanol based on recent shock tube/laser absorption experiments ⁴⁶⁴ <i>Subith S. Vasu¹, S. Mani Sarathy²</i> ¹ University of Central Florida ² KAUST	C-15 Prediction of biofuel ignition quality using a DCN ↔ RON interconversion tool ⁶²⁶ <i>F.M. Haas, F.L. Dryer</i> Princeton University
11:50	A-16 Experimental and computational study of a two-dimensional methyl butanoate flame <i>L.A. Kaufman, C.S. McEnally, D.D. Das, L.D. Pfefferle, B.A.V. Bennett, M.D. Smooke</i> Yale University		
12:10	LUNCH - Ballrooms A & B		
1:30	Bell South Auditorium Session Chair: R.A. Yetter Invited Speaker: Richard H. West, Northeastern University Title: Building detailed kinetic models of combustion chemistry		
	Session A-4: Laminar Flames Bell South Auditorium Session Chair: C. McEnally	Session B-4: Reaction Kinetics Ballroom C Session Chair: T. Farouk	Session C-4: New Technology Seminar Room II Session Chair: M. Renfro
2:40	A-17 Numerical analysis of extinction limits of counterflow flames: Effects of nozzle diameter and separation distance ³²² <i>R.F. Johnson, A.C. VanDine, G. Esposito, H.K. Chelliah</i> University of Virginia	B-17 Water-gas-shift equilibrium in diffusion flames and the effect of non-equilibrium elementary reactions ^{46:} <i>Wendong Wu, Richard L. Axelbaum</i> Washington University	C-17 Staged, pressurized oxy-combustion: Computational fluid dynamics simulations of a novel burner design ⁶³² <i>Fei Xia, Benjamin M. Kumfer, Bhupesh Dhungel, Richard L. Axelbaum</i> Washington University
3:00	A-18 Experimental and numerical studies of ion and electron concentrations in laminar methane-oxygen counterflow diffusion flames <i>Parth V. Shah, Alexei V. Saveliev</i> North Carolina State University 328	B-18 An analysis of the partial-equilibrium assumption for bimolecular reactions in counter-flow diffusion flames ⁴⁷⁶ <i>Wendong Wu, Richard L. Axelbaum</i> Washington University	C-18 An integrated approach for the design of a pilot scale oxy-coal combustion reactor using CFD and chemical equilibrium software ⁶³⁸ <i>Albio D. Gutiérrez, Steven L. Rowan, Ismail B. Celik</i> West Virginia University
3:20	BREAK - Corridor		

	Session A-4: Laminar Flames (cont.) Session Chair: C. McEnally	Session B-4: Reaction Kinetics (cont.) Session Chair: T. Farouk	Session C-4: New Technology (cont.) Session Chair: M. Renfro
3:50	A-19 An experimental study of fuel decomposition and hydrocarbon growth processes in laminar non-premixed methane air coflow flames doped with seven pentanol isomers""334 <i>Dhrubajyoti D. Das, Charles S. McEnally, Lisa D. Pfeifferle Yale University</i>	B-19 Dehydrogenation and dehydration activity in low-temperature gas-phase alcohol pyrolysis""483 <i>Patrick J. Fahey, Vikram Seshadri, Phillip R. Westmoreland North Carolina State University</i>	C-19 Studies of condensed-phase hypergolic reactions in a counter-flow stagnation reactor""644 <i>Pulkit Saksena, Srinivas Tadigadapa, Richard A. Yetter Pennsylvania State University</i>
4:10	A-20 Fuel similarity for laminar flames of C₅ to C₈ n-alkanes""33: <i>Peng Zhao, Wenkai Liang, Fujia Wu, Chung K. Law Princeton University</i>	B-20 Non-ideality of flow tube experiments for reaction kinetics""488 <i>T. Farouk¹, F.M. Haas², F.L. Dryer² ¹University of South Carolina ²Princeton University</i>	C-20 Improving performance with alkaline doped iron-based materials as oxygen carrier in chemical looping combustion""64: <i>Lu Liu, Michael R. Zachariah University of Maryland</i>
4:30	A-21 Species measurements in a low-pressure, fuel-rich JP-10/H₂ flat flame""346 <i>Vikram Seshadri, Wenjun Li, Phillip R. Westmoreland North Carolina State University</i>	B-21 Novel microflow tube reactor: n-butane pyrolysis and oxidation 4: 4 <i>U. Shrestha, G.P. Simms, M.J. Rahimi, B.G. Samacki, H.K. Chelliah University of Virginia</i>	C-21 Supercritical pyrolysis of dodecane with colloidal platinum-decorated graphene sheets""65: <i>Hyung Sub Sim¹, Richard A. Yetter¹, Daniel M. Dabbs², Ilhan A. Aksay² ¹Pennsylvania State University ²Princeton University</i>
4:50	A-22 An experimental and modeling study of formaldehyde and 1,3,5-trioxane flame"" chemistry""34; <i>Jeffrey S. Santner, Francis M. Haas, Frederick L. Dryer, Yiguang Ju Princeton University</i>	B-22 A CSP-based analysis of ethylene-air mixing and oxidation in a partially stirred reactor""4: 8 <i>G. Esposito, H.K. Chelliah University of Virginia</i>	C-22 Surrogate fuel evaluation for burner development for non-conventional industrial fuels ""66" <i>Vijaykant Sadasivuni, Hwan Ho Kim, Chendhil Periasamy Air Liquide</i>
5:20 – 6:30			
ESSCI General Member Meeting Bell South Auditorium (All Encouraged to Attend)			

Wednesday, October 16, 2013

Bell South Auditorium

Session Chair: F.L. Dryer

8:30 Invited Speaker: Tanvir Farouk, University of South Carolina
Title: Droplet combustion: "Cool Flames" in Space?

	Session A-5: Laminar Flames Bell South Auditorium Session Chair: G. Esposito	Session B-5: Reaction Kinetics Ballroom C Session Chair: R. West	Session C-5: Droplets and Spray Seminar Room II Session Chair: D.C. Haworth
9:40	A-23 Response of over-ventilated non-premixed flames to transverse flow perturbations ³⁵⁷ <i>Nicholas Magina, Timothy Lieuwen</i> <i>Georgia Institute of Technology</i>	B-23 A betweenness centrality method for chemical network analysis and mechanism reduction ^{4; 4} <i>Peng Zhao¹, Samuel M. Nackman¹, Tianfeng Lu², Chung K. Law¹</i> ¹ Princeton University ² University of Connecticut	C-23 Effectiveness of xenon as fire suppressant under microgravity combustion environment ⁶⁷² <i>M.E.A. Fahd¹, T. Farouk¹, F.L. Dryer²,</i> ¹ University of South Carolina ² Princeton University
10:00	A-24 Dynamics and morphology of colliding spherical flames ³⁶⁵ <i>Sheng Yang, Swetaprovo Chaudhuri, Delin Zhu, Chung K. Law</i> <i>Princeton University</i>	B-24 Auto-ignition of iso-octane at elevated pressures in a rapid compression machine ^{4; :} <i>G. Kukkadapu, C.-J. Sung, A.K. Das</i> <i>University of Connecticut</i>	C-24 Butanol droplet combustion: Detailed numerical modeling and microgravity experiments <i>T. Farouk¹, Y.C. Liu², M.E.A. Fahd¹, C.T. Avedisian², F.L. Dryer³</i> ¹ University of South Carolina ² Cornell University ³ Princeton University
10:20	BREAK – Corridor		
10:50	A-25 Effect of thermal expansion on flame propagation in channels with nonslip walls: Numerical and analytical consideration ^{36; 36} <i>Berk Demircok¹, Damir Valiev², Vyacheslav Akkerman¹</i> ¹ West Virginia University ² Princeton University	B-25 Single pulse shock tube study on the effects of double bond position in unsaturated hydrocarbons and fatty acid methyl esters ⁵²⁶ <i>Aleksandr Fridlyand¹, S. Scott Goldsborough^{1,2}, Kenneth Brezinsky¹</i> ¹ University of Illinois ² Argonne National Laboratory	C-25 Comparison of spray combustion for jet-A and diesel in a constant volume chamber ⁶⁹⁹ <i>Wei Jing¹, William L. Roberts^{1,2}, Tiegang Fang¹</i> ¹ North Carolina State University ² KAUST
11:10	A-26 Analysis of ethylene-oxygen combustion in micro-pipes ³⁷⁷ <i>Berk Demircok¹, Orlando Jesus Ugarte Almeyda¹, Vyacheslav Akkerman¹, Damir Valiev², Vitaly Bychkov³, Ming-Hsun Wu⁴</i> ¹ West Virginia University ² Princeton University ³ Umea University ⁴ National Cheng Kung University	B-26 Shock tube measurements of the reaction rates of OH with ketones at high temperatures ⁵³² <i>Jihad Badra¹, Ahmed Elwardany¹, Fethi Khaled¹, Subith S. Vasu², Aamir Farooq¹</i> ¹ KAUST ² University of Central Florida	C-26 Oxy-combustion of low-volatility fuel with high water content ^{6: 5} <i>Fei Yi, Richard L. Axelbaum</i> <i>Washington University</i>

	Session A-5: Laminar Flames (cont.) Session Chair: G. Esposito	Session B-5: Reaction Kinetics (cont.) Session Chair: R. West	Session C-5: Droplets and Spray (cont.) Session Chair: D.C. Haworth
11:30	A-27 Studies on the DC electric field effects on the combustion of fuel droplets ³⁸³ <i>Solomon Bengan, Tryfon T. Charalampopoulos</i> <i>Louisiana State University</i>		C-27 A first order approach to modeling fuel incidence angle of an air-blast injector for gas turbine combustion ⁶ ; <i>Kevin Matiko</i> <i>Embry-Riddle Aeronautical University</i>
11:50	ADJOURN Box Lunch – Corridor GE Tour (Depart at 1:30) <i>(Transport bus or car)</i>		

Additional Papers:

Toward Predictive CFD Models for Advanced Compression-ignition Engines: Accounting for Unresolved Turbulent Fluctuations^{6, 7}
D.C. Haworth

CFD Modeling of Industrial Fire Protection – Progress and Challenges⁷²³
Y. Wang

Low-Emissions Gas Turbine Combustion: Design Trends and Challenges⁷²⁹
K. McManus

Building Detailed Kinetic Models of Combustion Chemistry⁷³⁴
R. West

Droplet Combustion: “Cool Flames” in Space?⁷³⁹
T. Farouk