

**2018 SPRING TECHNICAL MEETING
EASTERN STATES SECTIONS OF THE COMBUSTION INSTITUTE
The Pennsylvania State University, Pennsylvania
March 4-7, 2018**

Sunday, March 4, 2018

17:00 – 20:00 Days Inn Foyer: Registration

13:00 – 16:00 108 Sackett Building: Cantera Workshop

15:30 – 17:30 Days Inn: ESSCI Executive Board Meeting

18:00 – 20:00 Days Inn Foyer: Welcome Reception

Monday, March 5, 2018

7:00 – 18:00 Days Inn Foyer: Registration

8:15 Main Hall: Welcome Remarks/Announcements

Jacqueline O'Connor, The Pennsylvania State University

Yuan Xuan, The Pennsylvania State University

8:30 Main Hall:

Plenary Lecture: William H. Green, Massachusetts Institute of Technology

Title: *Predicting Combustion Chemistry & Focusing on the Important Aspects*

Session Chair: Yuan Xuan, The Pennsylvania State University

9:30 – 9:45 Transition to Morning Session

	Reaction Kinetics I Room 1 Session Chair: M.P Burke	Oxygenates Room 2 Session Chair: F.M. Haas	Droplets Room 3 Session Chair: S.G. Tuttle
9:45	1A01: Evaluated rate constants for <i>i</i>-butane + H and CH₃: Shock tube experiments with Bayesian model optimization <i>L.A. Mertens, I.A. Awan, J.A. Manion</i> <i>National Institute of Standards and Technology</i>	1B01: Shock tube studies of methyl propanoate and methane kinetics <i>S. Jouzdani, D.M. Coomb, X. Zheng, B. Akhi-Kumgeh</i> <i>Syracuse University</i>	1C01: Three stage quasi-steady droplet burning behavior of <i>n</i>-alkane droplets at elevated pressure conditions: Hot, warm and cool flame combustion <i>T. Farouk¹, D. Dietrich², F.L. Dryer^{1,3}</i> ¹ <i>University of South Carolina</i> ² <i>NASA Glenn Research Center</i> ³ <i>Princeton University</i>

	Reaction Kinetics I Room 1 Session Chair: M.P. Burke	Oxygenates Room 2 Session Chair: F.M. Haas	Droplets Room 3 Session Chair: S.G. Tuttle
10:00	1A02: Kinetics of H atom addition to cyclopentane <i>J.A. Manion, I.A. Awan</i> <i>National Institute of Standards and Technology</i>	1B02: Shock tube and CO laser-absorption measurements during cyclopentanone oxidation <i>E. Ninnemann¹, S. Barak¹, O. Pryor¹, W.H. Green², K. Zhang³, W.J. Pitz³, S. Vasu¹</i> ¹ <i>University of Central Florida</i> ² <i>Massachusetts Institute of Technology</i> ³ <i>Lawrence Livermore National Laboratory</i>	1C02: Computational study of oscillatory cool flame dynamics for submillimeter sized n-heptane droplet <i>F.E. Alam¹, A.C. Aghdam¹, F.L. Dryer^{1,2}, T.I. Farouk¹</i> ¹ <i>University of South Carolina</i> ² <i>Princeton University</i>
10:15	1A03: Intramolecular phenyl migration in hexylbenzene radicals: An ab initio/TST study <i>S. Khanniche, W.H. Green</i> <i>Massachusetts Institute of Technology</i>	1B03: Premixed flame propagation in mixtures of cyclopentanone/air <i>G. Kim, B. Almansour, R. Blair, K. Ahmed, J. Kapat, S.S. Vasu</i> <i>University of Central Florida</i>	1C03: Motion of a merged drop upon impacting a liquid pool <i>A. Saha¹, Y. Wei^{1,2}, X. Tang¹, C.K. Law¹</i> ¹ <i>Princeton University</i> ² <i>Xi'an Jiaotong University</i>
10:30 – 11:00	BREAK – Days Inn Foyer		
	Reaction Kinetics II Room 1 Session Chair: C.B. Reuter	Sooting Tendencies Room 2 Session Chair: S.H. Won	Spray Flames Room 3 Session Chair: J.H. MacArt
11:00	1A04: A fully-automated kinetic mechanism lumping algorithm <i>L. Backer, P. Pepiot</i> <i>Cornell University</i>	1B04: Sooting tendencies of aromatic hydrocarbons with oxygencontaining side-chains <i>B.P. Beekley¹, C.S. McEnally¹, P.C. St. John², S. Kim², A. Jain³, H. Kwon³, Y. Xuan³, L.D. Pfefferle¹</i> ¹ <i>Yale University</i> ² <i>National Renewable Energy Laboratory</i> ³ <i>The Pennsylvania State University</i>	1C04: Droplet size and velocity measurements in a heptane/propane spray flame <i>B.T. Fisher, S.G. Tuttle, A.D. Tuesta</i> <i>Naval Research Laboratory</i>
11:15	1A05: Introducing a workflow for improving kinetic models: Case study using butanol <i>S.K. Sirumalla¹, M.A. Mayer², K.E. Niemeyer², R.H. West¹</i> ¹ <i>Northeastern University</i> ² <i>Oregon State University</i>	1B05: Numerical investigation of pressure dependence of yield sooting tendencies <i>Y. Xuan¹, C.S. McEnally², A. Jain¹, H. Kwon¹, L.D. Pfefferle²</i> ¹ <i>The Pennsylvania State University</i> ² <i>Yale University</i>	1C05: Droplet flamelet-generated manifold modeling for two-phase turbulent combustion <i>B.T. Bojko, P.E. DesJardin</i> <i>University at Buffalo, State University of New York</i>
11:30	1A06: An analytical jacobian generator for reduced chemical kinetic models involving quasi-steady-state assumptions <i>P. Sharma, H. Goyal, P. Pepiot</i> <i>Cornell University</i>	1B06: Sensitivity analysis and uncertainty propagation in numerical simulations of yield sooting tendencies <i>Y. Xuan, K. Mohhan, A. Jain, H. Kwon</i> <i>The Pennsylvania State University</i>	1C06: Reynolds-averaged Navier-Stokes simulations of a piloted heptane/propane spray flame <i>D.A. Kessler, B.T. Fisher, A.D. Tuesta, S.G. Tuttle</i> <i>Naval Research Laboratory</i>

	Reaction Kinetics II Room 1 Session Chair: C.B. Reuter	Sooting Tendencies Room 2 Session Chair: S.H. Won	Spray Flames Room 3 Session Chair: J.H. MacArt
11:45	1A07: ChemKED for profile-resolved data: A discussion of some salient data standard features <i>F.M. Haas¹, C.F. Goldsmith², M.P. Burke³, B.W. Weber⁴, K.E. Niemeyer⁵</i> ¹ Rowan University ² Brown University ³ Columbia University ⁴ University of Connecticut ⁵ Oregon State University	1B07: Analyzing the robustness of the yield sooting index as a measure of sooting tendency <i>M.J. Montgomery, D.D. Das, C.S. McEnally, L.D. Pfefferle</i> Yale University	1C07: A numerical investigation of the chemical kinetics in the low temperature oxidation process of n-heptane spray (I) <i>Y. Li¹, H. Ge², H. Li¹</i> ¹ West Virginia University ² Texas Tech University
12:00 – 13:30	Lunch Graduate Student Workshop – Room 4		
13:30 – 14:30	Main Hall – Glassman Lecture Invited Speaker: Wenting Sun, Georgia Tech Title: <i>The Effect of Ozone Addition on Combustion: What We Know and What We Don't</i> Session Chair: Paul Papas, UTRC		
	2:30 – 2:45 Transition to Afternoon Sessions		
	Reaction Kinetics III Room 1 Session Chair: M.E. Fuller	Sooting Flame Simulations Room 2 Session Chair: T. Grenga	New Devices Room 3 Session Chair: H. Goyal
14:45	1A08: Shock tube and kinetic modelling study of organo phosphorus compounds used as chemical weapon simulants <i>S. Neupane, F. Barnes, S. Barak, E. Ninnemann, Z. Loparo, A.E. Masunov, S.S. Vasu</i> University of Central Florida	1B08: A multi-moment sectional method to predict the soot size distribution <i>S. Yang, M.E. Mueller</i> Princeton University	1C08: A “scale-up” Swiss-roll combustor and its application in waste gas incineration <i>J. Crawmer¹, C.-H. Chen¹, B. Richard¹, H. Pearlman¹, P. Ronney², T. Edwards³</i> ¹ Advanced Cooling Technologies, Inc. ² The University of Southern California ³ Temple University
15:00	1A09: Carbon addition lowers initiation and iodine release temperatures from iodine oxide-based biocidal energetic materials <i>T. Wu, X. Wang, S. Holdren, M.R. Zachariah</i> University of Maryland	1B09: Subfilter transport modeling for large eddy simulation of turbulent nonpremixed sooting flames <i>S. Yang, J.K. Lew, M.E. Mueller</i> Princeton University	1C09: Swiss-roll JP-8 fuel reformer with direct center fuel injection and mixing chamber design <i>J. Crawmer¹, C.-H. Chen¹, B. Richard¹, H. Pearlman¹, P. Ronney²</i> ¹ Advanced Cooling Technologies, Inc. ² The University of Southern California

	Reaction Kinetics III Room 1 Session Chair: M.E. Fuller	Sooting Flame Simulations Room 2 Session Chair: T. Grenga	New Devices Room 3 Session Chair: H. Goyal
15:15	1A10: Thermochemistry and kinetic analysis on the reactions and mechanisms of CH₃SCH₂CH₃ with oxygen and OH radicals <i>G. Song, J.W. Bozzelli New Jersey Institute of Technology</i>	1B10: Simulations of soot formation in high-pressure transient spray flames <i>S. Ferreyro Fernandez, D.C. Haworth The Pennsylvania State University</i>	1C10: Microwave plasma processing of methane: Optical diagnostics and carbon characterizations <i>R. Vander Wal¹, A. Sengupta¹, E. Musselman², K. Zeller², G. Skoptsov² ¹The Pennsylvania State University ²H Quest Vanguard, Inc.</i>
15:30	1A11: Ion-molecule reactions relevant to the detection of atmospheric oxidized mercury by chemical ionization mass spectrometry <i>F.J. Guzman, M. Cooper, J. Antley, J. Bozzelli, A. Khalizov New Jersey Institute of Technology</i>	1B11: Large eddy simulations of staged pressurized oxy-combustion <i>F.N. Karaismail¹, A. Gopan², R.L. Axelbaum², I. Celik¹, B.M. Kumfer² ¹West Virginia University ²Washington University in St. Louis</i>	1C11: Development of a constant volume combustion chamber for material synthesis <i>M. Morovatiyan, M. Shahsavan, J.H. Mack University of Massachusetts, Lowell</i>
15:45 – 16:00	BREAK – Days Inn Foyer		
	Laminar Flames Room 1 Session Chair: V. Acharya	Soot Room 2 Session Chair: S. Yang	Coal and Biomass Room 3 Session Chair: X. Zhao
16:00	1A12: Double luminous zones in inverse laminar jet diffusion flames <i>Z. Wang¹, P.B. Sunderland¹, R.L. Axelbaum² ¹University of Maryland ²Washington University in St. Louis</i>	1B12: Reconciliation of carbon oxidation rates and activation energies based on changing nanostructure <i>M. Singh¹, C.K. Gaddam¹, R.L. Vander Wal¹, X. Chen², A. Yezerets², K. Kamasamudram² ¹The Pennsylvania State University ²Cummins, Inc.</i>	1C12: Nitrogen oxide evolution in oxy-coal combustion <i>S.K. Sirumalla, A. Panahi, A. Purohit, A. Baugher, Y.A. Levendis, R.H. West Northeastern University</i>
16:15	1A13: Low-temperature multistage diffusion flames <i>O.R. Yehia, C.B. Reuter, Y. Ju Princeton University</i>	1B13: Analysis of East Asian soot-based inksticks through Raman spectroscopy <i>J. Giaccari^{1,2}, J.H. Miller¹ ¹George Washington University ²Smithsonian Institution</i>	1C13: Effect of variability in biomass properties on biomass devolatilization <i>H. Goyal, P. Pepiot Cornell University</i>
16:30	1A14: Multi-modal counterflow flames under autoignitive conditions <i>T. Grenga, J.F. MacArt, M.E. Mueller Princeton University</i>	1B14: Informing TiRe-LII assumptions of soot nanostructure and optical properties for estimation of soot primary particle diameter <i>M. Singh, R.L. Vander Wal The Pennsylvania State University</i>	1C14: A study on pulverized coal ignition using a two-stage flat-flame burner with a transition from a reducing to oxidizing environment <i>A. Adeosun, D. Khatri, A. Gopan, Z. Yang, T. Li, R.L. Axelbaum Washington University in St. Louis</i>

	Laminar Flames Room 1 Session Chair: V. Acharya	Soot Room 2 Session Chair: S. Yang	Coal and Biomass Room 3 Session Chair: X. Zhao
16:45	1A15: Transient interactions between a premixed double flame and a vortex <i>C.B. Reuter¹, V.R. Katta², O.R. Yehia¹, Y. Ju¹</i> ¹ Princeton University ² Innovative Scientific Solutions, Inc.	1B15: Soot derivatization for source identification <i>M. Singh, R.L. Vander Wal</i> The Pennsylvania State University	1C15: Explosive dust characteristics evaluation of pulverized Pittsburgh coal using ASTM E1226-12a <i>J. Miller, P. Mulligan, C. Johnson</i> Missouri University of Science and Technology
17:00	1A16: Laminar flame propagation in supercritical hydrogen/air and methane/air mixtures <i>W. Liang, W. Li, C.K. Law</i> Princeton University	1B16: The effects of oxygenated fuels on soot particle nanostructure <i>J. Zhu, C.S. McEnally, L.D. Pfefferle</i> Yale University	1C16: Coal particle ignition in a combustion environment with a reducing-to-oxidizing transition <i>D. Khatri, A. Adeosun, A. Gopan, Z. Wang, R.L. Axelbaum</i> Washington University in St. Louis
17:15	1A17: Various regimes of premixed flame propagation in obstructed channels with both extremes open <i>A. Adebisi¹, E. Ridgeway¹, R. Alkandari¹, A. Cathreno¹, D. Valiev², V. Akkerman¹</i> ¹ West Virginia University ² Tsinghua University	1B17: Effects of hydrogen addition on the structure of <i>n</i>-dodecane laminar, co-flow flame <i>A. Makwana, M. Linevsky, S. Iyer, R. Santoro, T. Litzinger, J. O'Connor</i> The Pennsylvania State University	1C17: Predicting particle deposition for flow over a circular cylinder in combustion environments <i>A. Gopan, Z. Yang, R.L. Axelbaum</i> Washington University in St. Louis
17:30	1A18: Computational simulations of nonequidiffusive premixed flames in obstructed pipes <i>A. Adebisi¹, G. Idowu¹, D. Valiev², V. Akkerman¹</i> ¹ West Virginia University ² Tsinghua University	1B18: Soot characteristics of light naphtha in a constant volume combustion chamber using two-color pyrometry <i>Z. Wu¹, L. Wang¹, J.A. Badra², W.L. Roberts³, T. Fang¹</i> ¹ North Carolina State University ² Saudi Aramco ³ King Abdullah University of Science and Technology	1C18: Spectroscopic emission measurements and system level modeling of a two-stage wood-fired hydronic heater: Effects of non-homogeneous fuel decomposition <i>J.M. Weisberger, J.P. Richter, J.C. Mollendorf, P.E. DesJardin</i> University at Buffalo, the State University of New York
17:45	1A19: Transient ellipsoidal flames in microgravity <i>A. Markan¹, H.R. Baum¹, P.B. Sunderland¹, J.G. Quintiere¹, J.L. de Ris²</i> ¹ University of Maryland ² FM Global, retired	1B19: Quantification of nanostructure changes by HRTEM and fringe analyses during NO₂-O₂ oxidation <i>M. Srilomsak^{1,2}, M. Singh², K. Hanamura¹, R.L. Vander Wal²</i> ¹ Tokyo Institute of Technology ² The Pennsylvania State University	1C19: Experimental investigation of the stabilization and structure of turbulent cool diffusion flames <i>C.B. Reuter¹, O.R. Yehia¹, S.H. Won², M.K. Fu¹, K. Kokmanian¹, M. Hultmark¹, Y. Ju¹</i> ¹ Princeton University ² University of South Carolina
19:00 Young Faculty Mixer –Federal Taphouse			

Tuesday, March 6, 2018

8:00 – 16:00 **Days Inn Foyer: Registration**

8:15 **Main Hall: Announcements**
Jacqueline O'Connor, The Pennsylvania State University
Yuan Xuan, The Pennsylvania State University

8:30 **Main Hall:**
Plenary Lecture: Harsha K. Chelliah, University of Virginia
Title: *Hypersonic Propulsion: Challenges in Thermal Management and Flame Stabilization over a Range of Flow Conditions*
Session Chair: Daniel C. Haworth, The Pennsylvania State University

9:30 – 9:45 Transition to Morning Session

	Reaction Kinetics IV Room 1 Session Chair: G. Song	Fire - Instrumentation Room 2 Session Chair: A. Gopan	Turbulent Flames Room 3 Session Chair: C.E. Dumitrescu
9:45	2A01: A study of JP-10 pyrolysis by molecular beam mass spectrometry with comparison to literature model <i>G.P. Simms, H.K. Chelliah</i> <i>University of Virginia</i>	2B01: CMOS based high-speed camera pyrometry measurements for validation of upward flame spread modeling <i>S.S. Aphale, P.E. DesJardin</i> <i>University at Buffalo, State University of New York</i>	2C01: The effect of non-axisymmetric fuel staging on flame structure in a multiple-nozzle model turbine combustor <i>O. Sekulich, W. Culler, J. O'Connor</i> <i>The Pennsylvania State University</i>
10:00	2A02: Investigation of ethylene ozonolysis reaction's temporal behavior and products using plug flow reactor <i>B. Wu, X. Gao, W. Sun</i> <i>Georgia Institute of Technology</i>	2B02: Designing a gas sampling system for a 3 MW fire calorimeter using an experimental approach <i>J. Hashempour, R. Ranellone, A. Simeoni, N. Dembsey</i> <i>Worcester Polytechnic Institute</i>	2C02: The influence of mixedness on ignition for hydrogen direct injection in a constant volume combustion chamber <i>M. Shahsavan, M. Morovatiyan, J.H. Mack</i> <i>University of Massachusetts Lowell</i>
10:15	2A03: Catalytic ignition and pressure dependence of methane/air combustion over palladium oxide <i>R. Sui^{1,2}, W. Liang¹, J. Mantzaras², C.K. Law¹</i> ¹ Princeton University ² Paul Scherrer Institute	2B03: Flight test demonstration of LED-based fire sensors for space propulsion vehicles <i>A.C. Terracciano¹, K. Thurmond¹, M. Villar¹, J. Urso¹, E. Ninnemann¹, A. Parupalli¹, Z. Loparo¹, N. Demidovich², J.S. Kapat¹, S.S. Vasu¹</i> ¹ University of Central Florida ² FAA Office of Commercial Space Transportation	2C03: The effects of piloting on turbulent flame structure <i>R. Shupp¹, A. Tyagi¹, I. Boxx², S. Peluso¹, J. O'Connor¹</i> ¹ The Pennsylvania State University ² DLR, German Aerospace Center
10:30 – 11:00	BREAK – Days Inn Foyer		

	Reaction Kinetics V Room 1 Session Chair: T.I. Farouk	Pool Fires Room 2 Session Chair: B.T. Fisher	Turbulent Combustion Modeling Room 3 Session Chair: L. Backer
11:00	2A04: Impact of cyclo-alkanes on ignition propensity measured as derived cetane number in multi-component mixtures <i>D. Carpenter, S. Nates, S.J. Lim, F.L. Dryer, S.H. Won</i> <i>University of South Carolina</i>	2B04: In situ burn ignition testing methods and results for California crude oils <i>S.G. Tuttle, B.T. Fisher, C.J. Pfitzner, T.N. Loegel, K.M. Hinnant</i> <i>U.S. Naval Research Laboratory</i>	2C04: Challenges for large eddy simulation of partially premixed turbulent combustion using reduced-order manifold flame structure models <i>B.A. Perry, M.E. Mueller</i> <i>Princeton University</i>
11:15	2A05: Surrogate formation based on chemical functional group analysis <i>S. Nates, D. Carpenter, S.J. Lim, F. Dryer, S.H. Won</i> <i>University of South Carolina</i>	2B05: Evaluating foam degradation and fuel transport rates through novel surfactant firefighting foams for the purpose of AFFF perfluorocarbon replacement <i>K. Hinnant, A. Snow, S. Giles, R. Ananth</i> <i>U.S. Naval Research Laboratory</i>	2C05: Topologically conditioned chemical pathways for turbulent lean premixed n-dodecane/air flames <i>D. Dasgupta¹, W. Sun¹, M. Day², A.J. Aspden³, T. Lieuwen¹</i> <i>¹Georgia Institute of Technology</i> <i>²Lawrence Berkeley National Laboratory</i> <i>³Newcastle University</i>
11:30	2A06: Pyrolysis of fuel mixtures at supercritical conditions: A ReaxFF molecular dynamics study <i>S. Shabnam, C. Ashraf, A. Jain, Y. Xuan, A.C.T. van Duin</i> <i>The Pennsylvania State University</i>	2B06: Effect of low temperature wall on the extinction and fuel layer distribution of pool fires <i>C. Li¹, H.F. Farahani¹, R. Yang², A.S. Rangwala¹</i> <i>¹Worcester Polytechnic Institute</i> <i>²Tsinghua University</i>	2C06: On the accessed region of composition space in turbulent diffusion flames <i>A.S. Newale, Y. Liang, S.B. Pope, P. Pepiot</i> <i>Cornell University</i>
11:45	2A07: Fuel distillation affects spray flame blowout thresholds <i>J.A. Lefkowitz, F.M. Haas</i> <i>Rowan University</i>	2B07: Liquid-pool fire extinction characteristics of aqueous foams generated from fluorine-free surfactants <i>R. Ananth, S. Giles, K. Hinnant, X. Zhuang, A. Snow, J. Fleming, J. Farley</i> <i>U.S. Naval Research Laboratory</i>	2C07: A comprehensive model for non-adiabatic multi-modal combustion using physically-derived reduced-order manifolds <i>A.C. Nunno, M.E. Mueller</i> <i>Princeton University</i>
12:00 – 13:15	Lunch Diversity Workshop – Room 4		
	13:15 – 13:30 Transition to Afternoon Sessions		

	Reaction Kinetics VI Room 1 Session Chair: S. Khanniche	Solid Propellants and Explosives Room 2 Session Chair: S.S. Vasu	Turbulent Flames Room 3 Session Chair: J.W. Meadows
13:30	2A08: Addressing discrepancies in hydrogen abstraction by OOH radical via automatic transition state theory calculations <i>N. Harms, R.H. West</i> <i>Northeastern University</i>	2B08: Mechanism development of aqueous hydroxylammonium nitrate under thermal decomposition conditions <i>K. Zhang, S.T. Thynell</i> <i>The Pennsylvania State University</i>	2C08: DNS of cavity stabilized premixed turbulent flame with a high-order immersed boundary method <i>A.H. Rauch¹, K. Aditya², H. Kolla², J.H. Chen², H.K. Chelliah¹</i> ¹ <i>University of Virginia</i> ² <i>Sandia National Laboratories</i>
13:45	2A09: Multiscale informatics of reactions involved in H₂O₂ decomposition in the presence of dopants <i>C.E. LaGrotta, M.C. Barbet, L. Lei, M.P. Burke</i> <i>Columbia University</i>	2B09: Development of gas-phase reaction mechanism for ammonium perchlorate using quantum mechanics calculations <i>T. Chatterjee, S.T. Thynell</i> <i>The Pennsylvania State University</i>	2C09: Large eddy simulation and probability density function modelling of swirling Cambridge/Sandia turbulent stratified flame series <i>H. Turkeri, X. Zhao</i> <i>University of Connecticut</i>
14:00	2A10: Studies of pentane oxidation and pyrolysis in nanosecond-pulsed plasma discharges using in-situ laser diagnostics <i>A. Rousso¹, X. Mao^{1,2}, Q. Chen², Y. Ju¹</i> ¹ <i>Princeton University</i> ² <i>Beijing Jiaotong University</i>	2B10: Investigation into the structure-function relation of 3D printed energetic films: Single layer formulation study <i>M.C. Rehwoldt, H. Wang, N. Eckman, D. Kline, M.R. Zachariah</i> <i>University of Maryland</i>	2C10: Budgets of flame-conditioned second-order turbulence statistics in low and high Karlovitz number turbulent premixed jet flames <i>J.F. MacArt, T. Grenga, M.E. Mueller</i> <i>Princeton University</i>
14:15	2A11: Low-temperature oxidation of n-dodecane in a microflow tube reactor: Temperature and residence times effects <i>K. Dang, H.K. Chelliah</i> <i>University of Virginia</i>	2B11: Liquid-phase decomposition of RDX: Formation of oxy-s-triazine and 1,3,4-oxadiazole <i>L. Patidar, M. Khichar, S.T. Thynell</i> <i>The Pennsylvania State University</i>	2C11: Topology of local flame-flame interaction events in turbulent flames <i>A. Tyagi¹, I. Boxx², R. Shupp¹, S. Peluso¹, J. O'Connor¹</i> ¹ <i>The Pennsylvania State University</i> ² <i>DLR, German Aerospace Center</i>
14:30	2A12: Effects of <i>sp</i>² carbon on low-temperature oxidation of cyclic hydrocarbons <i>J.C. Davis¹, A.L. Koritzke¹, R.L. Caravan², M.G. Christianson¹, D.L. Osborn², C.A. Taatjes², B. Rotavera¹</i> ¹ <i>University of Georgia</i> ² <i>Sandia National Laboratories</i>	2B12: Computational study of condensed-phase kinetics during combustion of pure RDX <i>M. Khichar, L. Patidar, S.T. Thynell</i> <i>The Pennsylvania State University</i>	2C12: Cellular instability in expanding turbulent flames <i>Z. Liu, A. Saha, S. Yang, C.K. Law</i> <i>Princeton University</i>
14:45	2A13: The kinetic study of excited singlet oxygen atom O(¹D) reactions with acetylene <i>C. Yan, C. Teng, T. Chen, A. Rousso, G. Wysocki, Y. Ju</i> <i>Princeton University</i>	2B13: Impact of chemically termolecular reactions on the kinetics of energetic materials <i>R.E. Cornell, C.E. LaGrotta, M.C. Barbet, M.P. Burke</i> <i>Columbia University</i>	2C13: Numerical simulations of oxy-fuel premixed combustion in supercritical CO₂-diluted environment <i>A. Adebisi¹, V. Akkerman¹, K. Kemenov²</i> ¹ <i>West Virginia University</i> ² <i>Symplectic Research, Inc.</i>

15:00 – 15:30				BREAK – Days Inn Foyer			
NOx Kinetics Room 1 Session Chair: N. Harms		Refrigerants Room 2 Session Chair: P.B. Sunderland		Combustion Instabilities Room 3 Session Chair: W. Culler			
15:30	<p>2A14: On the relative importance of HONO versus HNO₂ in low-temperature combustion <i>M.E. Fuller, C.F. Goldsmith</i> <i>Brown University</i></p>	<p>2B14: An improved test method for refrigerant flammability limits in a 12 L vessel <i>D.K. Kim, A.E. Klieger, P.Q. Lomax, C.G. McCoy, J.Y. Reymann, P.B. Sunderland</i> <i>University of Maryland</i></p>	<p>2C14: Thermoacoustic linear stability model with porous media and mean flow effects <i>C. Dowd, J. Meadows</i> <i>Virginia Tech</i></p>				
15:45	<p>2A15: A computational investigation into the kinetics of NO + CH₂CCH and its effect on NO reduction <i>A.D. Danilack, C.F. Goldsmith</i> <i>Brown University</i></p>	<p>2B15: Deflagrations of mildly flammable refrigerant-air mixtures in closed volumes <i>K.C. Gottiparthi¹, P. Papas¹, V. Sankaran¹, P. Verma¹, R. Lord², L. Burns²</i> ¹<i>United Technologies Research Center</i> ²<i>Carrier Corporation</i></p>	<p>2C15: Thermoacoustic analysis with statistically based flame transfer function extracted from computational fluid dynamics <i>S. Sampathkumar, J.W. Meadows</i> <i>Virginia Tech</i></p>				
16:00	<p>2A16: Multidimensional numerical investigation of NO_x formation in a burner coupled flow tube configuration <i>S.F. Ahmed¹, A. Dasgupta², F.L. Dryer^{1,3}, T.I. Farouk¹</i> ¹<i>University of South Carolina</i> ²<i>Combustion Science and Engineering Inc.</i> ³<i>Princeton University</i></p>	<p>2B16: Predicted burning velocities of C1 and C2 hydrofluorocarbon refrigerant flames with air <i>G. Linteris, V. Babushok</i> <i>National Institute of Standards and Technology</i></p>	<p>2C16: Effects of transverse nozzle location on high-frequency transverse combustion instabilities in can combustors <i>V. Acharya, T. Lieuwen</i> <i>Georgia Institute of Technology</i></p>				
16:15	<p>2A17: Kinetic study of NO_x formation for synthetic natural gas combustion under gas turbine relevant conditions <i>F.E. Alam¹, S.F. Ahmed¹, F.L. Dryer^{1,2}, T.I. Farouk¹</i> ¹<i>University of South Carolina</i> ²<i>Princeton University</i></p>	<p>2B17: Development and validation of a mechanism for flame propagation in R-32/air mixtures <i>D.R. Burgess, Jr., J.A. Manion, R.R. Burrell, V.I. Babushok, M.J. Hegetschweiler, G.T. Linteris</i> <i>National Institute of Standards and Technology</i></p>	<p>2C17: Effects of the equivalence ratio transient durations on self-excited combustion instability time scales in a single nozzle combustor <i>X. Chen, W. Culler, S. Peluso, D. Santavicca, J. O'Connor</i> <i>The Pennsylvania State University</i></p>				
16:30 – 16:45 Short Break							
<p>16:45 – 17:45</p> <p>ESSCI General Member Meeting Main Hall <i>(All Encouraged to Attend)</i></p>							
<p>18:00 – 19:00</p> <p>Cocktail Hour Nittany Lion Inn – Boardroom Foyer</p>							
<p>19:00 – 22:00</p> <p>ESSCI Banquet Nittany Lion Inn – Boardroom</p>							

Wednesday, March 7, 2018

8:15 **Main Hall: Announcements**
Jacqueline O'Connor, The Pennsylvania State University
Yuan Xuan, The Pennsylvania State University

8:30 **Main Hall:**
Plenary Lecture: Erica Smithwick, The Pennsylvania State University
Title: Firescapes in the mid-Atlantic: Mismatches between social perceptions and prescribed re use
Session Chair: Jacqueline O'Connor, The Pennsylvania State University

9:30 – 9:45 Transition to Morning Session

	Reaction Kinetics VII Room 1 Session Chair: B. Rotovera	Fire - Modeling Room 2 Session Chair: A.S. Newale	SI Engines Room 3 Session Chair: A.C. Nunno
9:45	3A01: Accounting for real-gas effects in high-density combustion chamber <i>C. Zheng, B. Akih-Kumgeh</i> <i>Syracuse University</i>	3B01: Large eddy simulations of a methane-air turbulent line fire using flamelet combustion and non-gray gas radiation models <i>A. Marchand¹, V.M. Le^{1,2}, S. Verma¹, J. White¹, A.W. Marshall¹, T. Rogaume², F. Richard², J. Luche², A. Trouvé¹</i> ¹ <i>University of Maryland</i> ² <i>Université de Poitiers</i>	3C01: Role of low-temperature chemistry in detonation of <i>n</i>-heptane/oxygen/diluent mixtures <i>W. Liang¹, R. Mével², C.K. Law^{1,2}</i> ¹ <i>Princeton University</i> ² <i>Tsinghua University</i>
10:00	3A02: Effect of the presence of water molecules on syngas combustion: A ReaxFF molecular dynamics study <i>C. Ashraf, S. Shabnam, A.C.T. van Duin</i> <i>The Pennsylvania State University</i>	3B02: Memory optimization of a radiative heat transfer solver for fire simulations <i>A. Caratenuto, P. Zhang, B. Wu, X. Zhao</i> <i>University of Connecticut</i>	3C02: Effects of thermal and fuel stratifications and turbulence transport on knocking formation for dimethyl ether/air mixtures <i>T. Zhang¹, W. Sun¹, L. Wang², Y. Ju¹</i> ¹ <i>Princeton University</i> ² <i>Tsinghua University</i>
10:15	3A03: High-throughput screening for reactive and energy-transferring collider effects in complex-forming reactions <i>M.C. Barbet, K. McCullough, M.P. Burke</i> <i>Columbia University</i>	3B03: Development of 3D pyrolysis in FDS <i>M. Bruns¹, R. McDermott¹, S. Benkorichi², S. Hostikka³</i> ¹ <i>National Institute of Standards and Technology</i> ² <i>Omega Fire Engineering Ltd.</i> ³ <i>Aalto University</i>	3C03: Large-eddy simulations of a spark ignition IC engine <i>S.J. Kazmouz, D.C. Haworth</i> <i>The Pennsylvania State University</i>

10:30 – 11:00 **BREAK – Days Inn Foyer**

	Reaction Kinetics VIII Room 1 Session Chair: A. Makwana	Fire Room 2 Session Chair: A. Marchand	IC Engines Room 3 Session Chair: J.H. Mack
11:00	3A04: Dynamic evaluation of multi-component pressure dependence in multi-channel reactions: A case study of CH₃+OH system <i>L. Lei, M.P. Burke</i> <i>Columbia University</i>	3B04: Critical ignition conditions of structural materials by cylindrical firebrands <i>H. Salehizadeh, R.S.P. Hakes, M.J. Gollner</i> <i>University of Maryland</i>	3C04: Influence of turbulence-radiation interactions in engine radiation heat transfer <i>C. Paul¹, D.C. Haworth¹, S. Roy², M.F. Modest³</i> <i>¹The Pennsylvania State University</i> <i>²Marquette University</i> <i>³University of California, Merced</i>
11:15	3A05: Prompt dissociations of propyl radicals from OH + C₃H₈ and their role in combustion simulations <i>R. Sivaramakrishnan¹, C.F. Goldsmith², S.L. Peukert¹, J.V. Michael¹</i> <i>¹Argonne National Laboratory</i> <i>²Brown University</i>	3B05: Fire dynamics and forensic analysis of compartment fires <i>S.P. Kozhumal, G.E. Gorbett</i> <i>Eastern Kentucky University</i>	3C05: CFD-based non-equilibrium wall heat transfer models for engine-relevant conditions <i>A. Sircar, D.C. Haworth</i> <i>The Pennsylvania State University</i>
11:30	3A06: Explosion limits of H₂/CH₄/O₂ mixtures: Analyticity and dominant kinetics <i>W. Liang, Z. Liu, C.K. Law</i> <i>Princeton University</i>	3B06: A study of cavity effect on flame spread over kerosene-soaked sand bed <i>N. Mofidi, A.S. Rangwala</i> <i>Worcester Polytechnic Institute</i>	3C06: Combustion visualization in a single-cylinder heavy-duty CI engine converted to natural gas SI operation <i>J. Liu, C.E. Dumitrescu</i> <i>West Virginia University</i>
11:45	3A07: Measurement of methane autoignition delays in a shock tube under supercritical carbon dioxide conditions <i>M. Karimi, B. Ochs, W. Sun, D. Ranjan</i> <i>Georgia Institute of Technology</i>	3B07: The structure of a turbulent line fire subjected to cross-flow <i>S. Verma, A. Trouvé</i> <i>University of Maryland</i>	3C07: High load diesel engine-generator power improvement with advanced combustion modes <i>M. Walker, D.L. Prak, L. Hamilton, J. Cowart</i> <i>U.S. Naval Academy</i>
12:00	3A08: Color camera pyrometry and its impact in reaction visualization of energetic materials <i>D.J. Kline, R.J. Jacob, P.M. Guerieri, M.R. Zachariah</i> <i>University of Maryland</i>	3B08: Conditions for formation of the blue whirl <i>Y. Hu^{1,2}, S.B. Hariharan², M.J. Gollner², E.S. Oran²</i> <i>¹Tsinghua University</i> <i>²University of Maryland</i>	3C08: Compression-ignition of GDI sprays in a constant volume combustion chamber <i>L. Wang¹, F. Wang¹, W.L. Roberts², T. Fang¹</i> <i>¹North Carolina State University</i> <i>²King Abdullah University of Science and Technology</i>
12:15		3B09: Effects of ullage on combustion efficiency and plume entrainment of pit fires <i>V. Kimmerly, A.S. Rangwala</i> <i>Worcester Polytechnic Institute</i>	
12:30	Lunch 12:30 – 13:30 Adjourn The Pennsylvania State University Combustion Lab Tour Meet at 13:30 at the Atrium of Research East		

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