

# **Chemical and Physical Processes in Combustion**

**The 2003 Technical Meeting of the Eastern States  
Section of the Combustion Institute**



**The Pennsylvania State University  
University Park, PA  
October 26-29, 2003**



**Executive Committee of the Section, 2001-2003**

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	Moshe Lavid, <i>Energia</i>
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	Jerry M. Seitzman, <i>Georgia Institute of Technology</i>
	Mitchell D. Smooke, <i>Yale University</i>
	Stephen R. Turns, <i>The Pennsylvania State University</i>

**General Program**

<b>Sunday, October 26, 2003</b>		
<b>6:00 – 9:00 PM</b>	<b>Registration and Reception, Nittany Lion Inn</b>	
<b>Monday, October 27, 2003</b>		
<b>8:15 AM</b>	<b>Welcoming Remarks</b>	
<b>8:30 AM</b>	<b>I. Invited Speaker: "Experimental and Computational Tools for the Characterization of Nanoparticle Reactivity," Michael Zachariah, University of Minnesota</b>	
<b>9:30 AM</b>	<b>Sessions A-1, B-1, C-1</b>	
<b>12:30 PM</b>	<b>Lunch</b>	
<b>1:30 PM</b>	<b>II. Invited Speaker: "Nitric Oxide Formation and Removal in Non-premixed Flames," Volker Sick, University of Michigan</b>	
<b>2:30 PM</b>	<b>Sessions A-2, B-2, C-2</b>	
<b>Tuesday, October 28, 2003</b>		
<b>8:30 AM</b>	<b>III. Invited Speaker: "Chemical Microthrusters: Combustion Issues and Approaches," Richard A. Yetter, Vigor Yang, Ilhan A. Aksay, Frederick L. Dryer; The Pennsylvania State University, Princeton University</b>	
<b>9:30 AM</b>	<b>Sessions A-3, B-3, C-3</b>	
<b>12:30 PM</b>	<b>Lunch</b>	
<b>1:30 PM</b>	<b>IV. Invited Speaker: "Incipient Soot Formation and Growth," Hai Wang, University of Delaware</b>	
<b>2:30 PM</b>	<b>Sessions A-4, B-4, C-4</b>	
<b>5:30 PM</b>	<b>General Business Meeting</b>	
<b>6:30 PM</b>	<b>Reception</b>	
<b>7:30 PM</b>	<b>Banquet</b>	
<b>Wednesday, October 29, 2003</b>		
<b>8:30 AM</b>	<b>VI. Invited Speaker: "Combustion and Emissions from Biodiesel Fuels," Jon H. Van Gerpen, Iowa State University</b>	
<b>9:30 AM</b>	<b>Sessions A-5, B-5, C-5</b>	
<b>12:30 PM</b>	<b>Adjourn</b>	



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8:30 AM	I. Invited Speaker: "Experimental and Computational Tools for the Characterization of Nanoparticle Reactivity," Michael Zachariah, University of Minnesota	I.1
Session A1: Kinetics/ Fundamentals Chair: Edward Ritter, Villanova University		
9:30	1 "Wide Temperature Range Kinetics of the NH Reactions with H <sub>2</sub> and CO <sub>2</sub> ," A. Fontijn, S.M. Shamsuddin, P. Marshall, and W.R. Anderson, Rensselaer Polytechnic Institute, University of North Texas, US Army Research Laboratory	1
9:50	2 "Isodesmic Reactions for Transition States: Reactions of Cl Atoms with Methane and Halogenated Methanes," V. Knyazev, Catholic University of America, NIST	5
10:10	Break	
10:30	3 "Kinetics of the Reaction of the CCl <sub>2</sub> Biradical with NO," A.A. Shestov, S.A. Kostina, E.V. Shafir, I.R. Slagle, and V.A. Knyazev, Catholic University of America	9
10:50	4 "Thermochemical Properties, Pathway and Kinetic Analysis on the Reactions of Benzene with OH," C.C. Chen, J.W. Bozelli, and J.T. Farrell, New Jersey Institute of Technology, ExxonMobil	13
11:10	5 "Ab-Initio Study of the C <sub>6</sub> H <sub>5</sub> O + H Reaction: Visibility of the CO + C <sub>5</sub> H <sub>6</sub> Channel," A. V. Joshi, S.G. Davis, and H. Wang, University of Delaware	17
11:30	6 "Thermochemical and Kinetic Analysis of Otho-Xylene Oxidation Reactions," H. Sun and J.W. Bozelli, New Jersey Institute of Technology	21
11:50	7 "Energy Transfer Effects During the Multichannel Decomposition of Ethanol," W. Tsang, NIST	25

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Session B1: Fire Chair: Yiguang Ju, Princeton University		
9:30	8 "Water Mist Suppression of Propane-Air Flames: Modeling and Experimental Study," H.K. Chelliah, B.A. Williams, R.C. Mowrey, and J.W. Fleming, University of Virginia, Naval Research Laboratory	29
9:50	9 "Mitigation of Explosions in Enclosures using Water Mist," D. Schwer and K. Kailasanath, Naval Research Laboratory	33
10:10	Break	
10:30	10 "Wall-Vent Compartment Fire Behavior Under Limited Ventilation," Y. Utiskul and J.G. Quintiere, University of Maryland	37
10:50	11 "Zone Modeling of Wall Surface Heat Losses in Enclosure Fires," A. Trouvé, University of Maryland	41
11:10	12 "One-Dimensional Model of Wood Pyrolysis Including Char Surface Oxidation," N. Boonmee and J.G. Quintiere, University of Maryland	45
11:30	13 "New Fire-Safe Polysiloxane Polymers," A. Schoemann, P.R. Westmoreland, R.J. Farris, R. Kumar, A.C. Watterson, and L. Samuelson, University of Massachusetts, US Army Natick Soldier Center	49
11:50	14 "Developing Fire-Safe Polymers Using Milligram-Scale Test Methods," P.R. Westmoreland, H. Zhang, A. Schoemann, T. Inguilizian, and R.J. Farris, University of Massachusetts	53



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Session C1: Nanoparticles/Flame Synthesis			
Chair: Umit Koylu, University of Missouri-Rolla			
9:30	15	"Optimization of Flame Synthesis for Carbon Nanotubes Using Supported Catalyst," R. Vander Wal, L.J. Hall, and G.M. Berger, National Center for Microgravity Research	57
9:50	16	"Charge and Size Distribution Measurement of Nano-Sized Combustion Aerosols: Comparison with Theory," S.H. Kim, K.S. Woo, B.Y.H. Liu, and M. Zachariah, University of Minnesota	61
10:10		Break	
10:30	17	"Flame Synthesis of Titanium Oxide Nanoparticles," B. Zhao, J.R. McCormick, K. Bulanin, C.Y. Ni, J. Chen, and H. Wang, University of Delaware	65
10:50	18	"Demonstration of a Particle Feed System for Combustion Synthesis of Metal and Metal Oxide Materials," T.A. Miller, C.H. Chu, and M.S. Wooldridge, University of Michigan	69
11:10	19	"Electric Field Controlled High-Rate Synthesis of Vertically Aligned Carbon Nanotubes in Opposed Flow Oxy-Flame of Methane," W. Merchan-Merchan, A.V. Saveliev, and L.A. Kennedy, University of Illinois - Chicago	73
11:30	20	"Formation of Fullerenes in Opposed Flow Flames of Methane and Oxygen Enriched Air," M. Silvestrini, W. Merchan-Merchan, A. Saveliev, and L.A. Kennedy, University of Illinois - Chicago	77
11:50	21	"Study of Particle Inception Near and Below Sooting Limit by Scanning Mobility Particle Sizer," Z. Yang, B. Zhao, and H. Wang, University of Delaware	81

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Session A2: ScramJet/Turbines/Combustion of Solids Chair: Margaret S. Wooldridge, University of Michigan			
2:30	22	"Combustion Dynamics in a Scramjet Combustor with Transverse Fuel Injection," J.-Y. Choi, V. Yang, and F. Ma, Pusan National University, The Pennsylvania State University	85
2:50	23	"Effect of Swirl on Combustion Dynamics in a Lean-Premixed Gas-Turbine Combustor," Y. Huang and V. Yang, The Pennsylvania State University	89
3:10		Break	
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3:50	25	"Coal Dust Inerting and Post-Explosion Dust Sampling Research in a 1-m <sup>3</sup> Laboratory Chamber and an Experimental Mine," K. Cashdollar and J.E. Going, National Institute for Occupational Safety and Health, Fike Corporation	97
4:10	26	"Effects of Fuel Lewis Number on Flame Spread Over Solids," K. Tolejko, I. Feier, and J.S. T'ien, Case Western Reserve University	101
4:30	27	"Combustion Burn Time and Temperature Measurements of Ultra-Fine Metal Particles in a Shock Tube," N. Glumac, H. Krier, T. Bazyn, and R. Eyer, University of Illinois	105
4:50	28	"Numerical Modeling of Limiting Oxygen Index Apparatus: Effect of Gas Velocity on Oxygen Index for Film Type Fuels," A. Kumar and J.S. T'ien, Case Western Reserve University	109



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Chair: Andre Boehman, The Pennsylvania State University			
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2:50	30	"Theoretical Analysis of Flame Propagation in Small Scale Channels," Y. Ju, Princeton University	117
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3:30	31	"Multiphase Detonations in Tubes," S.A. Cheatham and K. Kailasanath, Naval Research Laboratory	121
3:50	32	"Thrust Chamber Dynamics of Airbreathing Pulse Detonation Engines," F. Ma, J.-Y. Choi, and V. Yang, The Pennsylvania State University	125
4:10	33	"Compact Pre-Detonator Design Criteria for Multi-Cycle PDE Applications," S.R. Saretto, S.-Y. Lee, C. Conrad, J. Brumberg, S. Pal, and R.J. Santoro, The Pennsylvania State University	129
4:30	34	"Anomaly Detection in a Generic Thermal Pulse Combustor," A. Mukhopadhyay, S. Datta, S. Gupta, A. Ray, and V. Yang, Jadavpur University, The Pennsylvania State University	133
4:50	35	"Thrust Measurements for a Pulse Detonation Engine Driven Ejector," R. Shehadeh, S.R. Saretto, S.-Y. Lee, S. Pal, and R.J. Santoro, The Pennsylvania State University	137

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3:10		Break	
3:30	38	"Hydroxyl Measurements in Interacting Edge Flames," A. Wason and M. Renfro, University of Connecticut	149
3:50	39	"On Low-Stretch Sub-limit Hydrogen Combustion," J.R. Nanduri, C.J. Sung, and J.S. T'ien, Case Western Reserve University	153
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4:30	41	"Computational and Experimental Study of Rich Partially Premixed Methane/Air Flames," B.V. Bennett, M.D. Smooke, A.N. Karpetis, and R.S. Barlow, Yale University, Sandia National Laboratory	161
4:50	42	"Dynamics of Edge Flames in Laminar and Turbulent Hydrogen-Air Counterflow," C.S. Yoo and Hong G. Im, University of Michigan	165



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Session A3: Kinetics/Modeling Chair: Joseph Bozelli, New Jersey Institute of Technology			
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10:30	45	"Experimental and Computational Study of Gas-Phase Oxidation of Hexafluoropropene with Molecular Oxygen," J.P. Dawson, M.A. Pingitore, and E.R. Ritter, Villanova University	177
10:50	46	"Development and Validation of a Skeletal Chemical Model for Methane and Propane Combustion," H.K. Chelliah, B.A. Williams, J. Fleming, University of Virginia, Naval Research Laboratory	181
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9:30	50	<b>"The Influences of Cylinder Wall Temperature and Equivalence Ratio on the First Cycle of a Gasoline Direct Injection Engine Cold Start," G.C. Frederick, J.V. Zello, and D.A. Santavicca, The Pennsylvania State University</b>	197
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11:10	54	<b>"Spray and Combustion of a DI Diesel Engine Operated with Biodiesel and B-20 Blended Fuel," M. Alam, J. Song, V. Zello, A. Boehman, E. Esen, and K. Miller, The Pennsylvania State University, ConocoPhillips Research</b>	213
11:30	55	<b>"A Hybrid Particle/Finite Volume PDF Method for Chemically Reacting Turbulent Flows: Computations of Autoignition in IC Engines," Y. Zhang and D.C. Haworth, The Pennsylvania State University</b>	217
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10:30	59	"Evaluation of OH Time-Series Asymmetries in Turbulent Nonpremixed Jet Flames," Y. Wang, M.W. Renfro, A. Chaturvedy, G.B. King, and N.M. Laurendeau, University of Connecticut, Purdue University	233
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11:10	61	"Large Eddy Simulation of Sandia Flame D," M.R.H. Sheikhi, T.G. Drozda, P. Givi, F.A. Jaber and S.B. Pope, University of Pittsburgh, Michigan State University, Cornell University	241
11:30	62	"Efficient Parallel Implementation of a Hybrid Finite-Volume/Particle Method for the PDF Equations of Turbulent Reactive Flows," R. Cao, D.A. Caughey, and S.B. Pope, Cornell University	245
11:50	63	"Development of a Photon Monte Carlo Method for DNS of Chemically Reacting Turbulent Flows," Y. Wu, M.F. Modest, and D.C. Haworth, The Pennsylvania State University	249

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2:50	65	"Soot Volume Fraction Measurements in Turbulent Non-Premixed Flames: A Comparison of In-Situ Laser and Ex-Situ Sampling Experiments," B. Yang, B. Hu, and U.O. Koynu, University of Missouri - Rolla	257
3:10		Break	
3:30	66	"Effects of Fuel Dilution on Soot Formation in Laminar Diffusion Flames," F. Xu, H. Mohammed, and R.H. Chen, University of Central Florida	261
3:50	67	"Towards a Comprehensive Model in Turbulent Non-Premixed Flames: Detailed Soot Calculations in Oxygen - Enriched Flames," L. Wang, D.C. Haworth, and S.R. Turns, The Pennsylvania State University	265
4:10	68	"Structure and Morphology of Soot Particles Formed in Opposed Flow Flames of Methane and Oxygen Enriched Air," W. Merchan-Merchan, A.V. Saveliev, and L.A. Kennedy, University of Illinois - Chicago	269
4:30	69	"Soot Nucleation in Laminar Premixed and Non-premixed Flames," A.M. El-Leathy, C.H. Kim, F. Xu, and G.M. Faeth, University of Michigan	273
4:50	70	"The Sooting Tendency of Prototype Advanced Thermally Stable Jet Fuels," Y. Yang, A.L. Boehman, and R.J. Santoro, The Pennsylvania State University	277



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Chair: Michael Renfro, University of Connecticut			
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2:50	72	"Selective Detection of C <sub>3</sub> H <sub>4</sub> and C <sub>6</sub> H <sub>6</sub> Isomers in Flames," M. Law, A. Morel, P.R. Westmoreland, T.A. Cool, and C. Taatjes, University of Massachusetts - Amherst, Cornell University, Sandia National Laboratories	285
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3:30	73	"Hyperspectral Infrared Imaging of Flames," W.T. Rawlins, D.B. Oakes, S.D. Wehe, D.X. Hammer, W.J. Marinelli, and M.G. Allen, Physical Sciences Inc.	289
3:50	74	"A Quantum Cascade Laser Sensor for SO <sub>2</sub> and SO <sub>3</sub> in Combustor Exhaust Streams," W.T. Rawlins, D.B. Oakes, D.M. Sonnenfroh, J.M. Hensley, M.L. Silva, and M.G. Allen, Physical Sciences Inc.	293
4:10	75	"In-Situ Optical Diagnostics for Measurements of Water Vapor Concentration and Temperature in PEM Fuel Cell," S. Basu, H. Xu, M.W. Renfro, and B.M. Cetegen, University of Connecticut	297
4:30	76	"Flame Ion Distribution in a Turbulent Premixed Combustor," B.T. Chorpeneing, J. Thornton, E.D. Huckaby, and E. Robey, National Energy Technology Laboratory, Parsons Project Services	301
4:50	77	"The Effects of Temperature and Quenching on Laser-Induced Fluorescence of Naphthalenes as JP-8 Tracers," S. A. Kaiser and M.B. Long, Yale University	305

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2:50	79	"Ignition of Al-Mg Mechanical Alloys," M.A. Trunov, M. Schoenitz, and E.L. Dreizen, New Jersey Institute of Technology	313
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3:30	80	"Oxidation Processes and Phase Changes in Metastable Al-Ti Alloys," X. Zhu, M. Schoenitz, and E.L. Dreizen, New Jersey Institute of Technology	317
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4:10	82	"Combustion of Aerosolized Spherical Al Powders and Flakes in Air," B.Z. Eapen, V.K. Hoffman, M. Schoenitz, and E.L. Dreizen, New Jersey Institute of Technology	325
4:30	83	"Characterization of Aluminum Powder Ignition," S. Mohan, M.A. Trunov, and E.L. Dreizen, New Jersey Institute of Technology	329
4:50	84	"AP / (N <sub>2</sub> +C <sub>2</sub> H <sub>2</sub> +C <sub>2</sub> H <sub>4</sub> ) Gaseous Fuel Diffusion Flame Studies," T.P. Parr, D.M. Hanson-Parr, M.D. Smooke, and R.A. Yetter, Naval Air Warfare Center, Yale University, The Pennsylvania State University	333



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Chair: Harsha Chelliah, University of Virginia			
9:30	85	"Computational and Experimental Study of a JP-8 Counterflow Diffusion Flame," J.A. Cooke, M. Bellucci, M.D. Smooke, A. Gomez, A. Violi, T. Faravelli, and E. Ranzi, Yale University, University of Utah, Politecnico di Milano	337
9:50	86	"A Computational Study of Near-Field Entrainment in Diesel Sprays Using a Two-Fluid Model," V. Iyer and J. Abraham, GE Global Research Center, Purdue University	341
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10:30	87	"An Investigation on the Burning Speed of JP10-Air Mixtures at Higher Temperature and Pressure," F. Parsinejad and M. Metghalchi, Northeastern University	345
10:50	88	"Effects of Fuel Composition on Soot Formation in a Turbulent Spray Burner," Y. Xia, T.A. Litzinger, S.Y. Lee, R.J. Santoro, and M. Linevsky, The Pennsylvania State University	349
11:10	89	"Development of a small scale combustor using a Si microfabricated electrospray atomizer," G. Paneda, X. Li, J. Klemic, M. Reed, and A. Gomez, Yale University	353
11:30	90	"Evaluation of Several Chemical Kinetics Mechanisms of Silane Ignition and Oxidation at Elevated Temperatures," D.M. Kalitan and E.L. Petersen, University of Central Florida	357

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9:50	92	"A Species Concentration Slip Model for Microscale Catalytic Reactions with Rarefied Gas Effect," B. Xu and Y. Ju, Princeton University	365
10:10		Break	
10:30	93	"Nonbuoyant Round Hydrocarbon-Fueled Laminar-Jet Diffusion Flames in Still Air," C. Aalburg, F.J. Diez, G.M. Faeth, P.B. Sunderland, D.L. Urban, and Z.-G. Yuan, University of Michigan, NASA Glenn Research Center	369
10:50	94	"A $D^n$ -Law for Nonane Droplet Combustion at Low Gravity," J.H. Bae and C.T. Avedisian, Cornell University	373
11:10	95	"The Effect of Gravity on the Shape, Propagation, and Stability of Cool Flames," H. Pearlman, M. Foster, and D. Karabacak, Drexel University	377



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<b>8:30 AM</b>		<b>V. Invited Speaker: "Combustion and Emissions from Biodiesel Fuels," Jon H. Van Gerpen, Iowa State University</b>	<b>V.1</b>
<b>Session C5: Flames II</b> Chair: Beth Bennett, Yale University			
9:30	96	"Chemiluminescence Measurements of Overall Heat Release Rates in Lean Premixed Turbulent Flames," <b>J. Lee, S. Miller, E. Gonzalez, and D.A. Santavicca, The Pennsylvania State University</b>	381
9:50	97	"Effect of Differential Diffusion on the Mutual Annihilation of Two Stoichiometric Premixed Hydrogen-Air Flames," <b>B. Ranganath and T. Echekki, North Carolina State University</b>	385
10:10		Break	
10:30	98	"Experimental Study of Fuel Decomposition and Hydrocarbon Growth Processes for Oxygenated Hydrocarbons: MTBE and Related Alkyl Ethers," <b>C.S. McEnally and L.D. Pfefferle, Yale University</b>	389
10:50	99	"Effect of Strain Rate on High-Pressure n-Heptane Autoignition in Counterflow," <b>S. Liu, J.C. Hewson, and J.H. Chen, Sandia National Laboratories</b>	393
11:10	100	"A Numerical Study on Combustion Phenomena in Meso-Scale Vortex Chambers," <b>Y. Wang, V. Yang, and R.A. Yetter, The Pennsylvania State University</b>	397
11:30	101	"An Experimental Study on Combustion Phenomena in Meso-Scale Vortex Chambers," <b>M.-H. Wu, R.A. Yetter, and V. Yang, The Pennsylvania State University</b>	401