CHEMICAL AND PHYSICAL PROCESSES IN COMBUSTION

1995 FALL TECHNICAL MEETING
THE EASTERN STATES SECTION OF THE COMBUSTION INSTITUTE
OCTOBER 16-18, 1995
WORCESTER POLYTECHNIC INSTITUTE
WORCESTER, MA
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Phillip R. Westmoreland
University of Massachusetts

Monday, October 16, 1995

Session A-1: Diagnostics I
Chairperson: K. C. Smyth, NIST


10:10 3. Gas Temperature Measurements by Stokes/Anti-Stokes Raman Thermometry in Spray Flames, A.N. Karpetis and A. Gomez, Yale University, New Haven, CT


11:30 6. Planar Imaging Applications in Sooting Turbulent Diffusion Flames, S.B. Gupta, T. Ni and R.J. Santoro, Penn State University, University Park, PA

Monday, October 16, 1995
Session B-1: Flames I
Chairperson: G. Patnaik, NRL


10:10 10. Star-Shaped Premixed Flames and Spatially Periodic Velocity Fields in Axisymmetric Counterflows, H. Lee and S.H. Sohrab, Northwestern University, Evanston, IL

10:50 11. The Fragile Structure of Partially Premixed Methane /Air vs. Air Counterflow Flames, M.A. Tanno, M.D. Snooke, Yale University, New Haven, CT, R.J. Osborne, T.M. Brown, and R.W. Pitz, Vanderbilt University, Nashville, TN

11:10 12. Reynolds and Lewis Number Effects in Unsteady Reactive Square Jets, F.F. Grinstein and K. Kailasanath, Naval Research Laboratory, Washington, DC


Monday, October 16, 1995
Session C-1: Chemical Kinetics I
Chairperson: A. Fontijn, RPI

9:30 15. Theoretical Rate Constants for the NH$_3$ + NO$_x$ = NH$_3$ + HNO$_x$ (x = 1,2) Reactions by Ab Initio MO/VTST Calculations, A.M. Mebel, E.W.G. Diau, M.C. Lin and K. Morokuma, Emory University, Atlanta, GA

9:50 16. Time-Dependent Solutions of the Master Equation for Chemically Activated Reactions, J.W. Peterson and P.R. Westmoreland, University of Massachusetts, Amherst, MA

10:10 17. O + NNH — A Possible New Route for NO$_x$ Formation in Flames, J.W. Bozzelli, New Jersey Institute of Technology, Newark, NJ, and A.M. Dean, Exxon Research and Engineering Co., Annandale, NJ

10:50 18. Ab Initio MO and RRKM Calculations for the Multichannel Rate Constants of the C$_2$H$_3$ + O$_2$ Reaction, A.M. Mebel, E.W.G. Diau, M.C. Lin and K. Morokuma, Emory University, Atlanta, GA

11:10 19. Analysis of Mono-Chloro Vinyl and Vinyl Radical Reactions with O$_2$, H.M. Chiang, T.H. Lay and J.W. Bozzelli, New Jersey Institute of Technology, Newark, NJ


Monday, October 16, 1995
Session A-2: Ignition and Detonations
Chairperson: S. Hochgreb, MIT

2:30 22. Dynamics Near Ignitions and Extinctions of Premixed H₂/Air Mixtures, S. Kalamitsanos and D.G. Vlachos, University of Massachusetts, Amherst, MA


4:10 26. Inhibition of Homogeneous Ignition by a Catalytic Surface, P.A. Bui, D.G. Vlachos and P.R. Westmoreland, University of Massachusetts, Amherst, MA


Monday, October 16, 1995
Session B-2: Models and Methods for Numerical Combustion
Chairperson: M. A. Tanoff, Yale University


3:10 31. Recent Developments of the Lewis PDF Solver, A.T. Norris, NASA Lewis Research Center, Cleveland, OH


4:50 35. Ordered Species List, Based on Valence Bonds, For Use in Hydrocarbon Combustion Models, E. Mankarios, M. Metghalchi, Northeastern University, Boston, MA, and J.C. Keck, MIT, Cambridge, MA
Monday, October 16, 1995

Session C-2: Fires, Flame Spread and Soot Radiation
Chairperson: V. Motiwalla, WPI

2:30 36. Large Eddy Simulations of Buoyant Plumes, W.E. Mell, A. Johnson, K.B. McGrattan and H.R. Baum, National Institute of Standards and Technology, Gaithersburg, MD

2:50 37. Prediction of Induced Radial Velocity Due to Vortical Structures in Pool Fires, T.A. Ahmed and B.M. Cetegen, University of Connecticut, Storrs, CT

3:10 38. Effects of Fire Size on Extinguishment Time and Acid Byproducts During Real Scale Halon Replacement Testing, A. Maranghides, R.S. Shenon, B.H. Black and W.D. Smith, Naval Research Laboratory, Washington, DC


4:50 42. Spectral Extinction Coefficients of Soot Aggregates from Turbulent Diffusion Flames, U.O. Küçüç, Yale University, New Haven, CT, and G.M. Faeth, Univ. of Michigan, Ann Arbor, MI

Tuesday, October 17, 1995

Session A-3: Unsteady and Pulsed Combustion
Chairperson: H. Johari, WPI

9:30 43. The Perfectly Stirred Pulsed Reactor, A.S. Feitelberg, GE Corporate Research and Development, Schenectady, NY

9:50 44. Dependence of a Helmholtz Pulse Combustor Performance and Operating Limits Upon Fuel Composition and Equivalence Ratio, A. Kushari, L. Rosen, J.I. Jagoda and B.T. Zinn, Georgia Institute of Technology, Atlanta, GA

10:10 45. Combustion Oscillation: Chemical Control Showing Mechanistic Link to Recirculation Zone Purge Time, R.S. Gemmell, G.A. Richards, M.J. Yip and T.S. Norton, Morganou Energy Technology Center, Morgantown, WV

10:50 46. Effect of Acoustic Oscillations on Sooty Flames, T. Kan, L. Rosen and J.I. Jagoda, Georgia Institute of Technology, Atlanta, Georgia

11:10 47. Active Control of Combustion Instabilities through Periodic Secondary Fuel Injection, C.M. Jones, F. Stone, W.P. Shih and D.A. Santavicca, Penn State University, University Park, PA


11:50 49. Flame Structure Evolution in an Unstable Lean Premixed Gas Turbine Combustor, W.P. Shih, J. Lee and D.A. Santavicca, Penn State University, University Park, PA
Tuesday, October 17, 1995

Session B-3: Soot Precursors
Chairperson: J. H. Miller, The George Washington University

9:30 50. Soot Suppressing Mechanisms of Ferrocene Additive in Laminar Hydrocarbon/Air Nonpremixed Flames, C.G. Megaridis, K.A. Jensen, J. Zhang and M.Y. Choi, University of Illinois at Chicago, Chicago, IL

9:50 51. Aromatic and Linear Hydrocarbon Concentration Measurements in a Non-Premixed Flame, C.S. McNally and L.D. Pfefferle, Yale University, New Haven, CT


11:10 54. Rapid Naphthalene Production from Allene and Toluene, M.B. Colket, United Technologies Research Center, East Hartford, CT

11:30 55. A Kinetic Model Describing Polyarene Growth, M.C. Masonjones and A.F. Sarofim, MIT, Cambridge, MA

11:50 56. The Rate of Carbonization of Soot Precursor Particles, R.A. Dobbins, G.J. Govatzidakis, W. Lu, A.F. Schwartzman, Brown University, Providence, RI, and R.A. Fletcher, National Institute for Standards and Technology, Gaithersburg, MD

Tuesday, October 17, 1995

Session C-3: Diagnostics II; Flames II
Chairperson: W. T. Ashurst, Sandia National Laboratories

9:30 57. Species Measurements in Laminar Diffusion Flames of Different Fuel Mixtures, D.C. Rapp, S. Seo and R.J. Santoro, Penn State University, University Park, PA


10:50 60. On the Burning Rate for Premixed Flames, F.C. Gouldin, Cornell University, Ithaca, NY


Tuesday, October 17, 1995

Session A-4: Droplets and Sprays; High Temperature Syntheses
Chairperson: B. M. Cetegen, University of Connecticut

2:30 64. Size Selective Dispersion of Droplets in an Isothermal Confined Mixing Layer, M.S. Tageldin and B.M. Cetegen, University of Connecticut, Storrs, CT

2:50 65. Computational and Experimental Study of Counterflow Spray Diffusion Flames, Y. D’Angelo, I. Silverman, L.P. Gao, A. Gomez and M.D. Smooke, Yale University, New Haven, CT

3:10 66. Co-flow Laminar Diffusion Flames of Monodisperse Sprays, Chen, G. and Gomez, A., Yale University, New Haven, CT

3:50 67. Droplet Vaporization and Combustion in Supercritical Flows, G.C. Hsiao and V. Yang, Penn State University, University Park, PA

4:10 68. Dispersion and Evaporation of Liquid Droplets in a Differentially-Heated Confined Mixing Layer, M.S. Tageldin and B.M. Cetegen, University of Connecticut, Storrs, CT

4:30 69. Synthesis and Morphological Evolution of Al₂O₃ Particles in Laminar Counterflow Diffusion Flames, Y. Xing, Ü. Ö. Köylü and D.E. Rosner, Yale University, New Haven, CT


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Tuesday, October 17, 1995

Session B-4: Solids and Propellants; Heterogeneous Combustion
Chairperson: H. F. Calcote, AeroChem Research Laboratories


3:10 73. Statistical Kinetics for Char Combustion and Carbon Burnout, R.H. Hurt, Sandia National Laboratories, Livermore, CA, E.G. Brebesh and D.J. Maloney, Morgantown Energy Technology Center, Morgantown, WV

3:50 74. An Eigenvalue Method for Computing the Burning Rates of RDX Propellants, K. Prasad, M.D. Smooke, Yale University, New Haven, CT, and R.A. Yetter, Princeton University, Princeton, NJ

4:10 75. Distributed Activation Energy Model of Heterogeneous Coal Ignition, J.C. Chen, North Carolina A&T State University, Greensboro, NC


Tuesday, October 17, 1995

Session C-4: Chemical Kinetics II
Chairperson: K. Brezinsky, Princeton University

2:30 78. Chloroform Pyrolysis and Oxidation: Experiment and Elementary Reaction Mechanism, T.H. Lay, Y.S. Won and J.W. Bozelli, New Jersey Institute of Technology, Newark, NJ

2:50 79. An Experimental Study of Benzene Oxidation at Fuel-lean and Stoichiometric Equivalence Ratio Conditions, Y. Chai and L.D. Pfefferle, Yale University, New Haven, CT

3:10 80. Kinetics Analysis on the Reaction of Neopentyl with Oxygen, R. Wei and J.W. Bozelli, New Jersey Institute of Technology, Newark, NJ

3:50 81. Detailed Reaction Modeling on Chlorodifluoromethane and 2-Chloro-1,1,1,2-Tetrafluoroethane Pyrolysis, J.J. DiFelice and E.R. Ritter, Villanova University, Villanova, PA

4:10 82. An Investigation of Phenoxy and Cyclopentadienyl Radical Kinetics through the Pyrolysis and Oxidation of Anisole, M. Pecullan, K. Brezinsky and I. Glassman, Princeton University, Princeton, NJ


4:50 84. Thermochemical Kinetic Analysis on the Reaction of Tertiary Butyl Radical with Oxygen and an Elementary Reaction Mechanism for Tertiary Butyl Oxidation Below 1200 K, C.J. Chen and J.W. Bozelli, New Jersey Institute of Technology, Newark, NJ

Wednesday, October 18, 1995

Session A-5: Waste Disposal and Pollutants
Chairperson: J. C. Hermanson, WPI


9:50 86. The Incineration of CH2Cl2 and CC14 in an Air-Staged Two Zone Turbulent Reactor, T.B. Salem, R.B. Barat, New Jersey Institute of Technology, Newark, NJ, and C.A. Bass, United States Military Academy, West Point, NY


11:30 90. Emissions of NOx and CO from Turbulent Jet Flames in a Crossflow, R.V. Bandaru and S.R. Turns, Penn State University, University Park, PA

Wednesday, October 18, 1995

Session B-5: Soot Formation and Growth
Chairperson: J. Howard, MIT

9:30 92. Modeling of Soot Coagulation and Aggregation at High-Pressure Conditions, A. Kazakov and M. Frenklach, Penn State University, University Park, PA

9:50 93. Analysis of Soot Surface Growth in a Laminar C_2H_4/Air Diffusion Flame, D.C. Rapp and R.J. Santoro, Penn State University, University Park, PA

10:10 94. Effects of Hydrodynamics on Soot Formation in Hydrocarbon-Fueled Laminar Opposed Jet Diffusion Flames, K.-C. Lin and G.M. Faeth, University of Michigan, Ann Arbor, MI

10:50 95. Soot Surface Growth by Acetylene and PAH in a Premixed Ethylene Flame, T.G. Benish, J.B. Howard and A.L. Laffleur, MIT, Cambridge, MA

11:10 96. Soot Threshold Measurements Using a Well-Stirred Reactor, F. Takahashi, J.W. Blust, J. Zelina, R.C. Striebich, University of Dayton Research Institute, Dayton, OH, and C.W. Frayne, Wright Laboratory, Wright-Patterson Air Force Base, OH


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Wednesday, October 18, 1995

Session C-5: Flame Suppression; Novel Combustion Topics
Chairperson: P. R. Westmoreland, University of Massachusetts


9:50 100. C_1 Fluoro- and Hydrofluorocarbon Effects on the Extinction Characteristics of Methane vs. Air Counterflow Diffusion Flames, M.A. Tsoffer, R.R. Dobbins, M.D. Smooke, Yale University, New Haven, CT, D.R.F. Burgess Jr., M.R. Zachariah, W. Tsang, National Institute of Standards and Technology, Gaithersburg, MD, and Westbrook, P.R., University of Massachusetts, Amherst, MA


11:30 104. Nitrous Oxide Anesthesia Creates Flammable Intestinal Gases, G. Sidebotham, F. Cantelmi, D. Stoffa, Cooper Union, New York, NY, G. Wolf and E. Fried, SUNY Health Science Center at Brooklyn, Brooklyn, NY