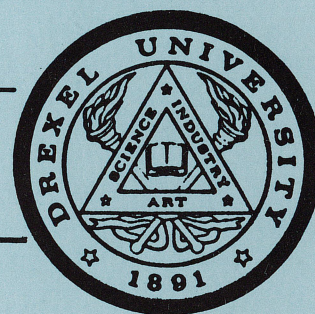
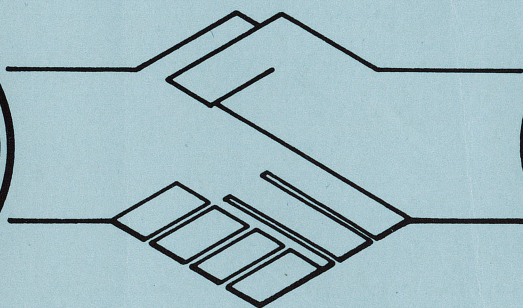
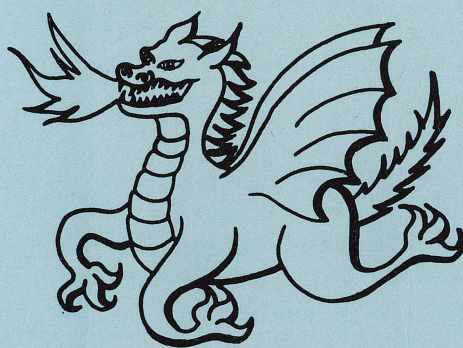


CHEMICAL AND PHYSICAL PROCESSES IN COMBUSTION



1985 FALL TECHNICAL MEETING

Eastern Section of The Combustion Institute
November 4 – 6, 1985, Philadelphia, Pennsylvania

Co-Hosted by:

The Pennsylvania State University

and

Drexel University

EASTERN SECTION OF THE COMBUSTION INSTITUTE - 1985 FALL TECHNICAL MEETING

SUNDAY, NOVEMBER 3, 1985, 6:30 - 9:00 p.m. -- REGISTRATION

MONDAY, NOVEMBER 4, 1985

8:30 a.m. A. Invited Speaker -- "Molecular Mixing in Turbulent Reacting Flow," W. A. Sirignano, University of California--Irvine.

Session A-1 Numerical Simulation and Modeling Turbulence

Chairperson: E. S. Oran
Naval Research Laboratory

9:20 a.m. 1. "Harmonic Modulation of a Confined Shear Layer," K. K. Ng and A. F. Ghoniem, Massachusetts Institute of Technology.

9:40 a.m. 2. "Time-Dependent Simulation of Small-Scale Turbulent Mixing and Reaction," H. R. Baum, D. M. Corley, and R. G. Rehm, National Bureau of Standards.

10:00 a.m. 3. "Nitric Oxide Formation and Turbulent Flame Structure," S. M. Correa, General Electric Company.

10:20 a.m. Coffee Break

10:40 a.m. 4. "Numerical Simulation of an Unstable Mixing Layer," F. F. Grinstein, E. S. Oran, and J. P. Boris, U.S. Naval Research Laboratory.

11:00 a.m. 5. "On the Modeling of Strong (Variable Density) Turbulent Buoyant Plumes and Ceiling Jets," M. A. Delichatsios, Factory Mutual Research Corporation.

11:20 a.m. 6. "Velocity-Density Correlations and Favre Averages Measured in a Premixed Turbulent Flame," A. Gulati and J. F. Driscoll, The University of Michigan.

11:40 a.m. Lunch Break

Session B-1 Laminar Flames
Chairperson: F. A. Williams
Princeton University

- 9:20 a.m. 7. "Enhancement of Premixed H₂/Air Flames with Photochemically Produced Radicals: Analytical Modeling," M. Lavid and J. G. Stevens, M. L. Energia, Inc., and C. K. Westbrook, Lawrence Livermore National Laboratory.
- 9:40 a.m. 8. "Multiphoton Ionization of Methyl Radicals in a Laminar Methane/Air Diffusion Flame," P. H. Taylor and K. C. Smyth, National Bureau of Standards.
- 10:00 a.m. 9. "Temperature, Soot, and Fuel Correlations in Laminar Diffusion Flames," L. R. Boedeker and G. M. Dobbs, United Technologies Research Center.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 10. "Effects of Geometry and Diffusive Transport on Premixed, Laminar Flame Propagation," K. Kailasanath, E. S. Oran, and G. Patnaik, U.S. Naval Research Laboratory.
- 11:00 a.m. 11. "Chemical Production Rates of Intermediate Hydrocarbons in Diffusion Flames: Preliminary Results for Acetylene," J. H. Miller, National Bureau of Standards.
- 11:40 a.m. Lunch Break

Session C-1 Soot
Chairperson: R. J. Santoro
National Bureau of Standards

- 9:20 a.m. 12. "Temperature Measurements in Sooting Flames by Optoacoustic Laser Deflection," S. A. Lawton, McDonnell Douglas Research Laboratories.
- 9:40 a.m. 13. "Acetylene Reactions in Methane-Oxygen Flames," J. M. Madson and M. A. Weissman, McDonnell Douglas Research Laboratories.
- 10:00 a.m. 14. "Effects of Alkaline-Earth and Similar Metal Additives on Soot in Flames," P. A. Bonczyk, United Technologies Research Center.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 15. "Soot Particle Growth and Transport in Laminar Diffusion Flames," R. J. Santoro, T. T. Yeh, J. J. Horvath, and H. G. Semerjian, National Bureau of Standards.
- 11:00 a.m. 16. "Some Observations on the Soot Formation Mechanism in Laminar Diffusion Flames at One and Two Atmospheres," W. L. Flower, Sandia National Laboratories, and C. T. Bowman, Stanford University.
- 11:20 a.m. 17. "Soot Particle Inception Rates," S. J. Harris, A. M. Weiner, and C. C. Ashcraft, General Motors Research Labs.
- 11:40 a.m. Lunch Break

MONDAY, NOVEMBER 4, 1985

1:20 p.m. B. Invited Speaker - "Hazards of Solid Propellants," T. L. Boggs, Naval Weapons Center.

Session A-2 Ignition, Combustion of Solids and Propellants
Chairperson: K. K. Kuo
The Pennsylvania State University

2:10 p.m. 18. "Ignition and Combustion Characteristics of Aluminum-Based Slurry Fuels," S. C. Wong and S. R. Turns, The Pennsylvania State University.

2:30 p.m. 19. "Further Experiments on the Combustion Behavior of Free Boron Slurry Droplets," F. Takahashi, F. L. Dryer and F. A. Williams, Princeton University.

2:50 p.m. 20. "Heats of Formation for Small Boron Compounds," M. Page, Naval Research Laboratory, and G. F. Adams, U.S. Army Ballistic Research Laboratory.

3:10 p.m. Refreshment Break

3:30 p.m. 21. "Erosive Burning of Stick Propellants, Theoretical Modeling," W. H. Hsieh and K. K. Kuo, The Pennsylvania State University.

3:50 p.m. 22. "Atmospheric Pressure Studies of Liquid Gun Propellant Drops in Hot Flows," R. A. Beyer, U.S. Army Ballistic Research Laboratory.

4:10 p.m. 23. "An Aerothermochemical Analysis of Carbon Particle Combustion," A. Makino and C. K. Law, University of California--Davis.

4:30 p.m. 24. "Radiative Ignition of Polymethylmethacrylate," T. X. Phuoc and P. Durbetaki, Georgia Institute of Technology.

4:50 p.m. Adjourn

5:00 p.m. Executive Committee Meeting

Session B-2 Atomization, Ignition, and Combustion of Fuel Sprays
Chairperson: G. M. Faeth
University of Michigan

2:10 p.m. 25. "Time Resolved Pulsed Spray Drop Sizing at Elevated Pressures," J. A. Drallmeier and J. E. Peters, University of Illinois at Urbana-Champaign.

2:30 p.m. 26. "Minimum Ignition Energies of Rich N-Heptane Fuel Sprays in the Transition Region," A. M. Danis, I. Namer, and N. P. Cernansky, Drexel University.

2:50 p.m. 27. "Spark Ignition of Monodisperse Aerosols," A. K. Singh and C. E. Polymeropoulos, Rutgers University.

3:10 p.m. Refreshment Break

3:30 p.m. 28. "Practical Modelling of Liquid Phase Temperature and Composition Transients in Vaporizing Droplets," D. G. Talley, University of Michigan, and S. C. Yao, Carnegie-Mellon University.

3:50 p.m. 29. "Observations of the Collision of Two Non-Burning and Burning Monodispersed Droplet Streams," N. Ashgriz, State University of New York at Buffalo.

4:10 p.m. 30. "Breakup Mechanisms of High Speed Liquid Jets," F. Ruiz and N. Chigier, Carnegie-Mellon University.

4:30 p.m. 31. "Tomographical Transformation of Spray Measurements," H. M. Zhu and N. Chigier, Carnegie-Mellon University.

4:50 p.m. Adjourn

5:00 p.m. Executive Committee Meeting

Session C-2 Kinetics - I
Chairperson: D. J. Seery
United Technologies Research Center

- 2:10 p.m. 32. "Reactions of Sodium Atoms at Elevated Temperatures by Time-Resolved Atomic Resonance Absorption Spectroscopy," P. Marshall and D. Husain, The University of Cambridge.
- 2:30 p.m. 33. "Ignition Delay Times for Hydrocarbon Oxidation Behind Reflected Shock Waves - A Preliminary Report," T. A. Brabbs, NASA Lewis Research Center, and T. F. Robertson, Case Western Reserve University.
- 2:50 p.m. 34. "Chemical-Kinetics Modeling for the Ignition and Flame Propagation in Idealized Sprays," S. K. Aggarwal, University of Illinois at Chicago.
- 3:10 p.m. Refreshment Break
- 3:30 p.m. 35. "Correlations Between Parameters of Global and Elementary Chemical Kinetic Mechanisms," R. A. Yetter, F. L. Dryer, and H. Rabitz, Princeton University.
- 3:50 p.m. 36. "A Comparison of the High-Temperature Oxidation Characteristics of Simple Alcohol Fuels," T. S. Norton and F. L. Dryer, Princeton University.
- 4:10 p.m. 37. "A Simple Method for Determining Global Activation Energies of Gaseous Fuel Air Mixtures," J. A. Clark, United Technologies, Pratt & Whitney.
- 4:30 p.m. 38. "Photochemical Effect on the Second Explosion Limit of H₂/O₂ System: Experimental and Analytical Results," M. Lavid, D. W. Blair, and J. G. Stevens, M. L. Energia, Inc.
- 4:50 p.m. Adjourn
- 5:00 p.m. Executive Committee Meeting

TUESDAY, NOVEMBER 5, 1985

8:30 a.m. C. Invited Speaker - "Fire Chemistry of Polymeric Materials," R. G. Gann, National Bureau of Standards.

Session A-3 Fire Research I
Chairperson: J. G. Quintiere
National Bureau of Standards

- 9:20 a.m. 39. "Transport Due to Flows with Opposing Buoyancy Arising in Room Fires," Y. Jaluria and D. Goldman, Rutgers University.
- 9:40 a.m. 40. "A PDF Method for Calculating Major Species Concentrations in Turbulent Fires," M. A. Delichatsios and M. K. Mathews, Factory Mutual Research Corporation.
- 10:00 a.m. 41. "An Experimental Study of the Transient Thermal Response of Unconfined Ceilings Above Fire Plumes," A. Woodhouse and C. H. Marks, University of Maryland, and L. Y. Cooper, National Bureau of Standards.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 42. "Heat Transfer in Compartment Fires Near Regions of Ceiling Jet-Wall Impingement," L. Y. Cooper, National Bureau of Standards.
- 11:00 a.m. 43. "A Model for a Burning Vertical Wall in the Stratified Atmosphere of a Compartment Fire," A. K. Kulkarni and J. J. Hwang, The Pennsylvania State University.
- 11:40 a.m. Lunch Break

Session B-3 Heterogeneous Combustion
Chairperson: W. A. Sirignano
University of California

- 9:20 a.m. 44. "An Asymptotic Theory of the Pyrolysis of Char-Forming Materials," I. S. Wichman, National Bureau of Standards, and A. Atreya, Michigan State University.
- 9:40 a.m. 45. "A Field Modeling Approach for Fires Over Large Liquid Pools: Boundary Layer Combustion Analysis," K. C. Adiga and D. E. Ramaker, The George Washington University, and P. A. Tatem and F. W. Williams, Naval Research Laboratory.
- 10:00 a.m. 46. "Exciplex Visualization Systems for Low Boiling Hydrocarbons," A. M. Murray and L. A. Melton, University of Texas at Dallas.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 47. "A Model for Vaporization and Devolatilization of a Coal-Water Slurry Droplet Under Intense Heating Conditions," S. S. Sandhu and E. A. Hess, University of Dayton.
- 11:00 a.m. 48. "An Experimental Study of Upward Turbulent Flame Spread on Wood Under External Radiation," K. Saito and F. A. Williams, Princeton University, and I. S. Wichman and J. Quintiere, National Bureau of Standards.
- 11:40 a.m. Lunch Break

Session C-3 Soot-Related Kinetics
Chairperson: F. L. Dryer
Princeton University

- 9:20 a.m. 49. "A Study of Soot Formation in Laminar Coflow-Air C₂ Diffusion Flames," A. Hamins, A. S. Gordon, and K. Seshadri, University of California--San Diego, and K. Saito, Princeton University.
- 9:40 a.m. 50. "Sooting Structure of a Counterflow Diffusion Flame: The Effect of Oxygen Addition to the Fuel," H. S. Hura and I. Glassman, Princeton University.
- 10:00 a.m. 51. "Soot Oxidation Kinetics," W. Felder, S. Madronich, and D. B. Olson, AeroChem Research Laboratories, Inc.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 52. "Multiple-Wavelength Pyrometer Measurement of Particle Size in Pulverized-Coal Flames," D. W. Mackowski, R. A. Altenkirch, and M. P. Menguc, University of Kentucky
- 11:00 a.m. 53. "Pyrolysis of Vinylacetylene," M. B. Colket, III, United Technologies Research Center.
- 11:20 a.m. 88. "Brownian Coagulation of Sub-Micron Smoke Aerosols," C. R. Kaplan, U.S. Naval Research Laboratory, and J. W. Gentry, University of Maryland.
- 11:40 a.m. Lunch Break

TUESDAY, NOVEMBER 5, 1985

- 1:20 p.m. D. Invited Speaker -- "Physical and Chemical Effects in Soot Formation," I. Glassman, Princeton University.

Session A-4 Fire Research II -- Flame Spread and Fire Growth
Chairperson: A. K. Kulkarni
The Pennsylvania State University

- 2:10 p.m. 54. "An Integral Analysis of the Equations of Wind-Aided Flame Spread," I. S. Wichman and H. R. Baum, National Bureau of Standards.
- 2:30 p.m. 55. "Diffusion Flame Stabilization at the Leading Edge of a Fuel Plate," C.-H. Chen and J. S. T'ien, Case Western Reserve University.
- 2:50 p.m. 56. "Flame Spread Over a Wall-Ceiling Corner," C.-P. Mao and A. C. Fernandez-Pello, University of California--Berkeley.
- 3:10 p.m. Refreshment Break
- 3:30 p.m. 57. "Burning Rate Measurements for Laminar Wall Fires Using Several Alcohols Burning in Air," S. F. Malary and J. K. Awad, Clarkson University.
- 3:50 p.m. 58. "Salt Water Modeling of Fire Induced Flows in a Multiroom Enclosure," K. D. Steckler, H. R. Baum, and J. G. Quintiere, National Bureau of Standards.
- 4:10 p.m. 59. "Hazards in a House Fire: Example of a Chair," M. M. Hirschler and G. F. Smith, BFGoodrich Chemical Company.
- 4:30 p.m. Adjourn
- 5:00 -
- 5:30 p.m. General Business Meeting. All Members Are Welcome.
- 6:30 p.m. Reception and Banquet

Session B-4 Ignition, Flame Stability, and Transients
Chairperson: B. T. Zinn
Georgia Institute of Technology

- 2:10 p.m. 60. "Experimental Investigations of Combustion Instabilities in Ramjets," U. G. Hegde, D. Reuter, B. R. Daniel, and B. T. Zinn, Georgia Institute of Technology.
- 2:30 p.m. 61. "Transient Cooling of a Hot Surface by Droplet Evaporation," A. K. Trehan and M. di Marzo, University of Maryland, and D. D. Evans, National Bureau of Standards.
- 2:50 p.m. 62. "Transition from Momentum- to Buoyancy-Controlled Turbulent Jet Diffusion Flames and Flame Height Relationships," M. A. Delichatsios, Factory Mutual Research Corporation.
- 3:10 p.m. Refreshment Break
- 3:30 p.m. 63. "Effect of Heat Release and Swirl on the Recirculation Within Swirl Stabilized Flames," V. Tangirala, R. H. Chen, and J. F. Driscoll, The University of Michigan.
- 3:50 p.m. 64. "Experimental and Analytical Results of Radiative Ignition in Premixed Hydrogen-Air Flows," M. Lavid and D. W. Blair, M. L. Energia, Inc.
- 4:10 p.m. 65. "An Exploration of the Chaotic Flame Propagation in Sprays," M. Queiroz and S. C. Yao, Carnegie-Mellon University.
- 4:30 p.m. Adjourn
- 5:00 -
- 5:30 p.m. General Business Meeting. All Members Are Welcome.
- 6:30 p.m. Reception and Banquet

Session C-4 Kinetics II

Chairperson: A. J. Fontijn
Rensselaer Polytechnic Institute

- 2:10 p.m. 66. "Bimolecular QRRK as a Tool for Combustion Modeling," P. R. Westmoreland, J. B. Howard, and J. P. Longwell, Massachusetts Institute of Technology, and A. M. Dean, Exxon Research and Engineering Company.
- 2:30 p.m. 67. "Unimolecular Reaction Pathways for Methylene Amidogen," M. J. Page, P. W. Saxe, B. H. Lengsfeld, and G. F. Adams, U.S. Army Ballistic Research Laboratory.
- 2:50 p.m. 68. "Preliminary Experiments with 1-Methylnaphthalene Near 1180K," T. A. Litzinger, K. Brezinsky, and I. Glassman, Princeton University.
- 3:10 p.m. Refreshment Break
- 3:30 p.m. 69. "Flow Reactor Oxidation Studies of the Extent of Reaction in Heptane/Iso-Octane Mixtures as a Function of Octane Number," S. P. Kennedy, K. Brezinsky, and F. L. Dryer, Princeton University.
- 3:50 p.m. 70. "Some Preliminary Observations on the High-Temperature Oxidation of Tert-Butyl Alcohol and Methyl Tert-Butyl Ether," T. S. Norton, F. L. Dryer, and K. Brezinsky, Princeton University.
- 4:10 p.m. Adjourn
- 5:00 -
- 5:30 p.m. General Business Meeting. All Members Are Welcome.
- 6:30 p.m. Reception and Banquet

WEDNESDAY, NOVEMBER 6, 1985

- 8:30 a.m. E. Invited Speaker -- "Concentration Measurements in Practical Flames by Laser-Saturated Fluorescence," N. Laurendeau, Purdue University.

Session A-5 Fire Research III -- Flame Radiation and Hazards
Chairperson: J. S. T'ien
Case Western Reserve University

- 9:20 a.m. 71. "Radiation Measurements of Large CH₄ Jet Diffusion Flames and the Effect of Water Sprays," B. J. McCaffrey, National Bureau of Standards.
- 9:40 a.m. 72. "Diffusion Flame Extinction at Small Stretch Rates: The Mechanism of Radiative Loss," J. S. T'ien, Case Western Reserve University.
- 10:00 a.m. 73. "Spectral Emission and Absorption Properties of Turbulent Ethylene/Air Diffusion Flames," J. P. Gore and G. M. Faeth, The University of Michigan.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 74. "Radiant Emission from Wall Fires," G. H. Markstein, Factory Mutual Research Corporation.
- 11:00 a.m. 75. "Sulfur Hexafluoride as a Surrogate for Verification of Destruction Removal Efficiency," M. L. Berger and C. Proctor, II, University of Florida.
- 11:20 a.m. 76. "Diffraction By and Transmission of a Detonation into a Bounding Explosive Layer," J. C. Liu, J. J. Liou, M. Sichel, and C. W. Kauffman, The University of Michigan.
- 11:40 a.m. Lunch Break

Session B-5 Diagnostics

Chairperson: N. P. Cernansky
Drexel University

- 9:20 a.m. 77. "Investigation of Integral Transform Techniques for Laser Diffraction Particle Size Analysis," J. H. Koo and E. D. Hirleman, Arizona State University.
- 9:40 a.m. 78. "Interference to CARS in Highly-Sooting Flames from C_2 Absorption," G. M. Dobbs, L. R. Boedeker, and A. C. Eckbreth, United Technologies Research Center.
- 10:00 a.m. 79. "Visualization of Jet Flames," L-D. Chen, The University of Iowa, and W. M. Roquemore, Air Force Wright Aeronautical Laboratories.
- 10:20 a.m. Coffee Break
- 10:40 a.m. 80. "Optimization of a Droplet Sizing Apparatus for in situ Measurements," D. L. Dietrich, I. Namer, and N. P. Cernansky, Drexel University.
- 11:00 a.m. 81. "CARS Spectroscopy of the Reaction Zone of CH_4/N_2O and Nitramine Propellant Flames," L. E. Harris, U.S. Army Armament Research Development Center.
- 11:20 a.m. 82. "Development of an Intensified Digital Line Camera System for Real-Time Line Measurements in Turbulent Flows," W. M. Pitts, National Bureau of Standards.
- 11:40 a.m. Lunch Break

WEDNESDAY, NOVEMBER 6, 1985

- 1:20 p.m. F. Invited Speaker -- "High Temperature Reactor Studies of Homogeneous Elementary Reactions," A. Fontijn, Rensselaer Polytechnic Institute.

Session A-6 Practical Combustion Devices

Chairperson: A. M. Mellor
Drexel University

- 2:10 p.m. 83. "Performance Characteristics of Helmholtz Type Pulsating Combustors," S. H. Ku, X. C. Cheng, B. R. Daniel, J. I. Jagoda, and B. T. Zinn, Georgia Institute of Technology.
- 2:30 p.m. 84. "Experimental Measurement of Particulate Emissions from a Deisel Operated with Particulate-Laden Intake Air," R. Gibbs, R. Whitby, and R. Johnson, New York State Department of Environmental Conservation.
- 2:50 p.m. 85. "The Design and the Characterization of a Fluidized Bed Combustor for Toxic Waste Incineration Research," R. T. Clawson, I. Namer, N. P. Cernansky, and R. J. Tidona, Drexel University.
- 3:10 p.m. Adjourn

Session B-6 Pollutants
Chairperson: M. B. Colkert, III
Princeton University

- 2:10 p.m. 86. "HC Emissions Modeling: Partial Burn Effects," G. A. Lavoie, A. A. Adamczyk, E. W. Kaiser, J. W. Cooper, and W. G. Rothschild, Ford Motor Company.
- 2:30 p.m. 87. "Particle-Size Effects on the Distribution of Fuel Nitrogen in One-Dimensional Coal-Dust Flames," K. C. Midkiff, R. A. Altenkirch, and K. Li, University of Kentucky.
- 2:50 p.m. 89. "Hydrogen Cyanide Decomposition and Reaction in an Electric Discharge," R. S. Sheinson and M. E. Fraser, U.S. Naval Research Laboratory.
- 3:10 p.m. Adjourn

Molecular Mixing in Turbulent Reacting Flow

by

William A. Sirignano
University of California, Irvine

Turbulent combustion occurs in any combustor or burner with a sufficiently high mass flow since Reynolds number tends to increase as mass flow increases. Turbulence will affect the transport rate, the mixing rate, and the chemical rate; therefore, it has significant effect upon the energy and species conversion rates and pollutant formation rates.

The large turbulent eddies transport reactants, products, and heat over the larger length scales but, by themselves, do not cause the gases to mix completely. The eddies will result in a mixed gas when resolved on a scale larger than the smallest eddy. However, when resolved on a smaller scale, the turbulent eddies result in a stratified gas; molecular diffusion is required to complete the mixing process. Clearly, for a diffusion flame, chemical reaction cannot begin until the reactants are mixed on the scale of the molecular mean free path. Similarly, in the premixed case, molecular diffusion of heat must eliminate the stratification of the temperature of the mixed reactants before rapid chemical reaction can occur.

Simplified models of turbulent combustion have been created that either assume that chemical kinetics is rate-controlling or that the mixing is rate-controlling and the mixing rate is determined by the characteristic time of the largest eddy in a cascade process. In either case, the overall conversion rate will not depend upon a Reynolds number; chemical kinetics rates depend upon a Damkohler number and the large-eddy rate depends on neither number. The time for molecular diffusion across the smallest eddy scale depends directly upon that length scale. The smallest eddy length scale decreases as Reynolds number increases so, if molecular mixing is a controlling factor, we can expect to see a Reynolds number dependence. Therefore, the appearance of a Reynolds number dependence for the conversion rate indicates that molecular mixing is one of the rate-controlling factors and perhaps the controlling factor.

Experimental studies in both a plug flow reactor⁽¹⁾ and a mixing layer configuration⁽²⁾ have indicated Reynolds number dependencies. Some calculations^(3,4), although performed with ad hoc models of molecular mixing, do indicate a Reynolds number effect. For these reasons, it is most worthwhile to develop accurate and informative models of molecular mixing.

Turbulent reacting flows can be studied by various analytical approaches. Many second-order closure studies have been performed to determine both velocity and scalar properties. Several studies have been performed that employ a second-order approach for the hydrodynamic variables and a probability density function (pdf) approach for the scalar variables. Some theories use assumptions about the pdf in order to assist in closure with