

# Outputs and Interactions– Physical and Chemical Properties Division FY 03

## 1. Publications

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- Watts, L.A., ***“Vapor-Liquid Equilibrium of Mixed Solvent Electrolyte Solutions: Measurements and Models,”*** Proc. Spectrum 2002 Conf., Reno, NV, August 4-8, 2002 (2003).
- Watts, L.A., ***“Fluid Properties Simulation Challenge. Recommendations for Problem II(c): 2-Propanol Density,”*** Fluid Phase Equil. (in press).
- Watts, L.A., ***“Fluid Properties Simulation Challenge. Recommendations for Problem II(d): Diethanol Amine Density,”*** Fluid Phase Equil. (in press).
- Watts, L.A., ***“Fluid Properties Simulation Challenge. Recommendations for Problem II(e): 1,2,3-Trichloropropane Density,”*** Fluid Phase Equil. (in press).
- Watts, L.A., ***“Fluid Properties Simulation Challenge. Recommendations for Problem II(f): Triethylene Glycol Density,”*** Fluid Phase Equil. (in press).
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## 2. Talks

- Andersen, W.C., "**Kinetics of Carbonyl Sulfide Hydrolysis: Studies in Propane and Other n-alkanes**," 225th American Chemical Society National Meeting, New Orleans LA, March 23, 2003.
- Andersen, W.C., "**Kinetics of Carbonyl Sulfide Hydrolysis in Propane and Light n-alkanes**," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 24, 2003.
- Andersen, W.C., "**Non-invasive Vapor Liquid Equilibrium Measurements**," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 27, 2003.
- Archer, D.G., "**Adiabatic Calorimetric Determination of Properties of Standard Reference Materials for Calibration of Differential Scanning Calorimetry**," 58<sup>th</sup> Annual Calorimetry Conference, Laie, HI, July 28, 2003. Invited.
- Bruno, T.J., "**Adsorption Thermodynamics of Natural Gas Odorants on Surrogate Soil Surfaces**," GTI Conference on Natural Gas Quality and Odorization, Orlando FL, October 2, 2002.
- Bruno, T.J., "**Pitfalls of the Copper Strip Corrosion Test**," GTI Conference on Natural Gas Quality and Odorization, Orlando FL, October 3, 2002.
- Bruno, T.J., "**Decomposition of Fluids used for the Organic Rankine Cycle**," National Renewable Energy Laboratory, Golden CO, December 12, 2002. Invited.
- Bruno, T.J., "**The Copper Strip Corrosion Test: Background, Pitfalls and Improvements**," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 24, 2003.
- Bruno, T.J., "**A Vapor Entraining Magnetic Mixer for Equilibrium, Reaction and Extraction Applications**," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 26, 2003.
- Bruno, T.J., "**Quantifying Vapor-Soil Interactions using Surrogate Soil Stationary Phases in Gas Chromatography**," Rocky Mountain Conference on Analytical Chemistry, Denver CO, July 29, 2003.
- Chirico, R.D., Diky, V.V., Wilhoit, R.C. and Frenkel, M., "**Global Submission and Validation of Experimental Thermodynamic Data using Guided Data Capture (GDC) Software: Benefits to Authors, Journals, and Data Users**," 225<sup>th</sup> American Chemical Society National Meeting, New Orleans LA, March 2003.
- Chirico, R.D., "**TRC Data Entry Facility: Linking the Global Network of Experimentalists and Users of Thermodynamic Data**," 3rd Annual NIST/TRC Consortium Workshop, NIST, Boulder CO, June 2003.

- Chirico, R.D., Diky, V.V., Wilhoit, R.C. and Frenkel, M., ***“Global Submission and Validation of Experimental Thermodynamic Data Using Guided Data Capture (GDC) Software,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 2003.
- Chirico, R.D., Diky, V.V., Wilhoit, R.C. and Frenkel, M., ***“Global Submission, Validation, and Dissemination of Experimental Thermodynamic Data Using Guided Data Capture (GDC) Software and ThermoML XML-based formats: Benefits to Authors, Journals, and Data Users,”*** 58<sup>th</sup> Annual Calorimetry Conference, Laie, HI, July 2003.
- Cafiero, M.L., ***“Nonadiabatic Studies of Molecules: Structures and Electrical Properties,”*** Department of Chemistry and Physics, University of North Florida, Jacksonville, FL, January 30, 2003.
- Chaka, A.M., ***“How Scientific Computing, Databases, and Knowledge Management can Enable Advances and New Insight in Chemical Technology,”*** National Academy of Science, Washington, DC, October 31, 2002. Invited.
- Chaka, A.M., ***“Surface Structure and Reactivity in a Complex Environment,”*** Department of Chemistry, University of North Texas, Denton, TX, March 28, 2003. Invited.
- Chaka, A.M., ***“How Scientific Computing can Enable Technical Decision Making in the Chemical Industry,”*** Rohm & Haas, Spring House, PA, April 10, 2003. Invited.
- Chaka, A.M., ***“How Scientific Computing can Enable Technical Decision Making in the Chemical Industry,”*** 3M, St. Paul, MN, April 17, 2003.
- Chaka, A.M., ***“Predicting Metal Oxide Surface Structures and Reactivity in a Complex Environment,”*** 3M, St. Paul, MN, April 17, 2003. Invited.
- Chaka, A.M., ***“Quantum Mechanics and the Automobile,”*** Howard University, Washington, DC, April 22, 2003. Invited.
- Chaka, A.M., ***“Metal Oxide Surface Chemistry,”*** Daresbury Laboratory, United Kingdom, May 12, 2003. Invited.
- Chaka, A.M., ***“Predicting Chemical and Physical Properties and Reactivity for Industrial Applications,”*** 15<sup>th</sup> Symp. on Thermophysical Properties, Boulder, CO, June 24, 2003. Invited.
- Chaka, A.M., ***“Validation of Computational Methods,”*** Army Research Office Workshop on “Tools for Condensed Phase Computational Chemistry,” University of Delaware, Newark, DE, May 28, 2003. Invited.
- Chaka, A.M., ***“Computation of Chemical and Physical Properties,”*** MERCURY - Computational Chemistry Summer Conference, Hamilton College, Hamilton, NY, July 31, 2003. Invited.
- Chaka, A.M., ***“How Scientific Computing, Databases, and Knowledge Management can Enable Advances and New Insight in Chemical Technology,”*** American Chemical Society National Meeting, New York, NY, September 7, 2003. Invited.
- Chaka, A.M., ***“Industrial Fluid Simulation Challenge,”*** American Chemical Society National Meeting, New York, NY, September 10, 2003.
- Chaka, A.M., ***“Dissociation of Oxygen and Water at Metal Oxide Surfaces: Role of the Surface and Surrounding Environment,”*** ACS National Meeting, New York, NY, September 10, 2003.
- Fahr, A., ***“Pressure Effects on Radical-Radical Reactions; Implications to the Modeling of Planetary Atmospheres,”*** NASA’s Division of Planetary Sciences Meeting, Birmingham, AL, October 8, 2002.

- Fahr, A., ***“Pressure and Temperature Effects on Product Channels of the Propargyl (HCCCH<sub>2</sub>) Combination Reactions, Formation of the “First Ring,”*** Combustion Research Facility/Sandia National Laboratories, May 21, 2003. Invited.
- Fahr, A., ***“Experimental Kinetics Mechanistic Investigations and of Hydrocarbon Radicals Relevant to Combustion Modeling,”*** Combustion Contractor’s Meeting of the Chemical Sciences Division, The Department of Energy, Tahoe City, Reno, NV, May 26, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V., Dong, Q., Frenkel, S., Franchois, P.R., Embry, D.L., Teague, T.L., Marsh, K.N. and Wilhoit, R.C., ***“New Process for Delivery of Experimental Thermophysical and Thermochemical Property Data,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 24, 2003.
- Frenkel, M., ***“Overview of TRC Activities over 2002-2003 Period,”*** 3<sup>rd</sup> (Twelfth) NIST/TRC Consortium Annual Workshop, Boulder CO, June 26, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V., Dong, Q., ***“ThermoML – XML-Based Approach for Storage and Delivery of Thermodynamic Data,”*** 58<sup>th</sup> Calorimetry Conference, Honolulu HI, July 29, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V. and Dong, Q., ***“ThermoML – New Approach for Thermodynamic Data Communications,”*** 226<sup>th</sup> ACS National Meeting, New York NY, September 10, 2003.
- Frenkel, M., ***“Overview of TRC Activities over 2002-2003 Period,”*** 3<sup>rd</sup> (Twelfth) NIST/TRC Consortium Annual Workshop, Boulder CO, June 26, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V., Dong, Q., Frenkel, S., Franchois, P.R., Embry, D.L., Teague, T.L., Marsh, K.N. and Wilhoit, R.C., ***“New Process for Delivery of Experimental Thermophysical and Thermochemical Property Data,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 24, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V., Dong, Q., ***“ThermoML – XML-Based Approach for Storage and Delivery of Thermodynamic Data,”*** 58<sup>th</sup> Calorimetry Conference, Honolulu HI, July 29, 2003.
- Frenkel, M., Chirico, R.D., Diky, V.V. and Dong, Q., ***“ThermoML – New Approach for Thermodynamic Data Communications,”*** 226<sup>th</sup> ACS National Meeting, New York NY, September 10, 2003.
- Friend, D.G., ***“Establishing Benchmarks for the First Industrial Fluids Simulation Challenge,”*** AIChE 2002 Annual Meeting, Indianapolis IN, November 3, 2002. Invited.
- Friend, D.G. and Frenkel, M., ***“ThermoML: XML-based Data Exchange Format from NIST Thermodynamics Research Center,”*** Report to the DIPPR Project 991 Steering Team, DIPPR Annual Meeting, Indianapolis IN, November 4, 2002. Invited.
- Friend, D.G., ***“Thermophysical Properties of Real Fuels,”*** Workshop on Combustion Simulation Databases for Real Transportation Fuels, Gaithersburg MD, September 4, 2003. Invited.
- Gonzalez, C.A., ***“Electronic Structure Rearrangements as a Source of Negative Differential Resistance in Molecules,”*** 6<sup>th</sup> Engineering Foundation Conferences on Molecular-Scale Electronics, Key West, FL, December 16, 2002.
- Gonzalez, C.A., ***“Critical Issues in the Application of Quantum Chemistry in Computational Kinetics,”*** 26<sup>th</sup> American Chemical Society National Meeting, New York, NY, September 10, 2003.
- Harvey, A.H., ***“Method for Estimating the Dielectric Constant of Natural Gas Mixtures,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 23, 2003.

- Harvey, A.H., ***“Aqueous Solubility of Volatile Nonelectrolytes,”*** IAPWS Annual Symposium, Vejle, Denmark, August 27, 2003. Invited.
- Harvey, A.H. and Lemmon, E.W., ***“Method for Estimating the Dielectric Constant of Natural Gas Mixtures,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 23, 2003.
- Huie, R.E., ***“Precise Kinetic Measurements on OH Reactions: Curvature in Arrhenius Plots,”*** International Symposium on Combustion and Atmospheric Pollution, St. Petersburg, Russia, July 8, 2003.
- Irikura, K.K., ***“Computational Chemistry: Not Theory, Not Experiment. Is it Science?,”*** Chemistry Department, University of Tennessee, Knoxville, TN, September 25, 2003.
- Irikura, K.K., ***“Groping Toward ab Initio Mass Spectrometry,” Chemical and Analytical Sciences Division,”*** Oak Ridge National Laboratory, Knoxville, TN, September 26, 2003.
- Kurylo, M.J., ***“A Kinetic Study of the Reaction of Hydroxyl Radicals with H<sub>2</sub> Over the Temperature Range 200K to 480K,”*** Gordon Conference on Atmospheric Chemistry, Big Sky, MT, September 8, 2003.
- Kurylo, M.J., ***“The Current Operational Status of and Future Plans for the Network for the Detection of Stratospheric Change,”*** Annual Meeting of the Scientific Steering Group for the Stratospheric Processes and their Role in Climate (SPARC) Project of the World Climate Research Program, Frankfurt, Germany, September 25, 2003.
- Kurylo, M.J., ***“Strategic Thrusts within NASA’s Atmospheric Composition Research Focus Area: Overlap with SPARC Initiatives,”*** 11<sup>th</sup> Session of the Scientific Steering Group for the Stratospheric Processes and their Role in Climate (SPARC) Project of the World Climate Research Program, Frankfurt, Germany, September 25, 2003.
- Kurylo, M.J., ***“NASA’s Plans for Sub-Orbital Science for the Validation of Aura and Other Satellites,”*** 11<sup>th</sup> Session of the Scientific Steering Group for the Stratospheric Processes and their Role in Climate (SPARC) Project of the World Climate Research Program, Frankfurt, Germany, September 26, 2003.
- Laesecke, A., ***“Who Discovered the Triple Point and When?”*** Department of Chemical Engineering, University of Wyoming, Laramie WY, April 21, 2003. Invited.
- Laesecke, A., ***“James Thomson and the Continuity of the Solid, Liquid, and Gaseous State,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 23, 2003.
- Laesecke, A., ***“Viscosity Measurements and Model Comparisons for the Refrigerant Blends R410A and R507A,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 25, 2003.
- Lemmon, E.W. and Starling, K., ***“Speed of Sound and Related Thermodynamic Properties Calculated from the AGA Report No. 8 Detail Characterization Method Using a Helmholtz Energy Formulation,”*** American Gas Association Conference and Biennial Exhibition, Orlando FL, April 28, 2003.
- Lemmon, E.W. and Span, R., ***“Short Fundamental Equations of State for Industrial Fluids,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 25, 2003.
- Lemmon, E.W., McLinden, M.O. and Huber, M.L., ***“The REFPROP Database for the Thermophysical Properties of Fluids,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 25, 2003.
- Lemmon, E.W. and Jacobsen, R.T., ***“A New Functional Form and Fitting Techniques for Equations of State with Application to Pentafluoroethane (HFC-125),”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 25, 2003.

- Linstrom, P.J., *"The NIST Chemistry WebBook: A Chemical Data Resource on the Internet,"* 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder, CO, June 24, 2003.
- Linstrom, P.J., *"Transitioning to a Structure Based Identification System,"* American Chemical Society National Meeting, New York, NY, September 10, 2003.
- Linstrom, P.J., *"Towards a Universal Physical Property Data Index,"* American Chemical Society National Meeting, New York, NY, September 8, 2003.
- Magee, J.W., *"Advances in Thermophysical Property Research on Ionic Liquids, Ionic Liquid Mixtures, and a Comprehensive Database,"* Panel Discussion, 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 26, 2003. Invited.
- Magee, J.W., *"Physical Properties and a Comprehensive Data Retrieval System for Ionic Liquids,"* 226<sup>th</sup> National Meeting of the American Chemical Society, as part of the Green Chemistry Symposium, New York City, NY, September 7, 2003.
- Mallard, W.G., *"The Use of AMDIS to Automate GC/MS Analysis,"* DuPont Protein Research Labs, St. Louis, MO, October 21, 2002.
- Mallard, W.G., *"AMDIS – Blinded Software for Automatic Analysis,"* International Workshop on the Analysis of Chemicals Related to the Chemical Weapons Convention, Helsinki, Finland, September 9, 2003.
- Manion, J.A., *"A Single Pulse Shock Tube Study of C<sub>2</sub>Cl<sub>6</sub> Decomposition: Are the Kinetics Consistent with the Proposed Thermochemistry of C<sub>2</sub>Cl<sub>6</sub> and C<sub>2</sub>Cl<sub>5</sub>?"* Third Joint Meeting of The Combustion Institute, University of Chicago, Chicago, IL, March 17, 2003.
- Matheu, D.M., *"New, Computer-Discovered Pathways for Methane and Ethane Pyrolysis,"* American Chemical Society National Meeting, New York, NY, September 9, 2003.
- McLinden, M.O., *"Apparatus for Wide-Ranging, High-Accuracy Fluid p-r-T Measurements Based on a Compact Two-Sinker Densimeter,"* 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 26, 2003.
- McLinden, M.O., *"The REFPROP Database for the Thermophysical Properties of Refrigerants,"* 20<sup>th</sup> International Congress of Refrigeration, Washington DC, August 19, 2003.
- Mikaia, A.I., *"Computer Assisted Quality Control of the NIST/NIH/EPA Mass Spectral Library,"* Eastern Analytical Symposium and Exposition, Somerset, NJ, November 21, 2002.
- Mikaia, A.I., *"Computer-Enhanced Evaluation Procedures for the NISR/EPA/NIH Mass Spectral Library,"* 16<sup>th</sup> Int. Mass Spectrometry Conf., Edinburgh, UK, September 4, 2003.
- Miller, K.E., *"Measurements at the Boundary: Investigations of Interfacial Properties of Industrial Systems,"* with T. J. Bruno, Baxter Healthcare Corporation, Round Lake IL, October 7, 2002.
- Miller, K.E., *"Sorption of Fuel Gas Odorants on Soils,"* Creighton University, Omaha NE, November 21, 2002.
- Miller, K.E., *"Measurements at the Boundary: Investigation of Interfacial Properties of Industrial and Environmental Systems,"* University of Denver, Denver CO, December 12, 2002.
- Miller, K.E., *"Sorption of Fuel Gas Odorants on Soils,"* United States Naval Academy, Annapolis, MD, January 13, 2003.

- Miller, K.E., ***“Sorption of Fuel Gas Odorants on Soils,”*** University of Northern Colorado, Greeley CO, February 21, 2003.
- Miller, K.E., ***“Sorption of Fuel Gas Odorants on Clay Surfaces by Gas Chromatography,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 24, 2003.
- Miller, K.E., ***“Evaluation of Clay Adsorbents by Liquid Chromatography,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder CO, June 25, 2003.
- Miller, K.E., ***“Clay Adsorbent Evaluation by Liquid Chromatography,”*** Rocky Mountain Conference on Analytical Chemistry, Denver CO, July 29, 2003.
- Mountain, R.D., ***“Molecular Dynamics of Liquids,”*** University of Pittsburgh, Pittsburgh, PA, May 14, 2003.
- Mountain, R.D., ***“Introduction to Molecular Dynamics,”*** 14<sup>th</sup> Advanced Cement Based Materials/NIST Computer Modelling Workshop, NIST, Gaithersburg, MD, June 12, 2003.
- Neta, P., ***“Reaction Kinetics in Ionic Liquids Studied by Pulse Radiolysis,”*** Physical and Chemical Properties Division, NIST, Gaithersburg, MD, February 20, 2003.
- Neta, P., ***“Pulse Radiolysis Studies of Reaction Kinetics in Ionic Liquids,”*** 23<sup>rd</sup> Miller Conference on Radiation Chemistry, Bialowieza, Poland, September 8, 2003.
- Orkin, V.L., ***“Photochemistry at Lithography Wavelengths,”*** Third Annual Technology Roadmap Workshop at Extraction Systems Inc., Wellesley, MA, June 9, 2003.
- Orkin, V.L., ***“Precise Measurements of Rate Constants for OH Reactions of Atmospheric Interest,”*** Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia, September 14, 2003.
- Radebaugh, R., ***“Alternative Refrigeration Technologies,”*** Low-Power Cryocooler Workshop, Amsterdam, The Netherlands, April 1, 2003. Invited.
- Radebaugh, R., ***“A Review of Cryocoolers,”*** Toshiba Corporation, Tokyo, Japan, April 18, 2003.
- Radebaugh, R., ***“Cryocoolers for Super Conductors,”*** Challenges of Applied Cryoelectrics II, WE-Heraeus-Workshop, Wilburg, Germany, May 27, 2003. Invited.
- Radebaugh, R., ***“Micro Cryocoolers,”*** Micro Cryogenic Coolers Workshop, Defense Advanced Research Projects Agency, Mystic CT, July 15, 2003. Invited.
- Radebaugh, R., ***“Improved Regenerators for Cryocoolers,”*** Interagency Energy Conversion Engineering Conference, Portsmouth VA, August 20, 2003. Invited.
- Radebaugh, R., ***“Optimization of Inertance Tubes,”*** Cryogenic Engineering Conference/International Cryogenic Engineering Conference, Anchorage AK, September 24, 2003.
- Radebaugh, R., ***“Experimental Measurements and Model Verification of Inertance Tubes,”*** Cryogenic Engineering Conference/International Cryogenic Engineering Conference, Anchorage, AK, September 25, 2003.
- Rainwater, J., ***“Virial Coefficients for Hard Spheres Immersed in Hard Rod Solutions,”*** 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder, CO, June 24, 2003.

- Rainwater J., "Issues of Forum 2000, Three Years Later," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder, CO, June 25, 2003. Invited.
- Rainwater, J., "**Hard Dumbbell Free Energy via the Fluctuating Cell Model**," 15<sup>th</sup> Symposium on Thermophysical Properties, Boulder, CO, June 25, 2003.
- Shen, V.K., "**Computational and Theoretical Investigation of Mechanical Strength in Glasses and Superheated Liquids**," Statistical Physics/Molecular Simulation Seminar, NIST, Gaithersburg, MD, January 8, 2003.
- Shen, V.K., "**Mechanical Properties of Glasses via the Energy Landscape**," Johns Hopkins University/Department of Physics, Baltimore, MD, March 26, 2003.
- Simmons, V., "**Molecular Dynamics Results on the Surface Tension of Three Binary Fluid Mixtures**," Annual American Physical Society Meeting, Austin, TX, March 3, 2003.
- Stein, S.E., "**An Automated Method for verifying Structure-Spectral Consistency based on Ion Thermochemistry**," 16<sup>th</sup> Int. Mass Spectrometry Conf., Edinburgh, UK, September 4, 2003.
- Stein, S.E., "**Open Standards for Chemical Information**," 226<sup>th</sup> American Chemical Society Fall Meeting, New York, NY, September 10, 2003.
- Stein, S.E., "**Open Standards for Chemical Information**," The IUPAC Chemical Identifier and XML Data Dictionaries Projects Creon Lab Control, Cologne, Germany, October 6, 2003.
- Stein, S.E., "**Open Standards for Chemical Information**," The IUPAC Chemical Identifier and XML Data Dictionaries Projects German Chemical Society Annual Meeting, Munich, Germany, October 8, 2003.
- Stein, S.E., "**An Open Standard for Chemical Structure Representation – The IUPAC Chemical Identifier**," Chemical Informatics Conference, Nimes, France, October 22, 2003.
- Tsang, W., "**Progress in the Development of Combustion Kinetics Databases for Liquid Fuels Codatata**," 2002-Frontiers of Scientific and Technical Data, Montreal, Canada, October 2, 2002.
- Tsang, W., "**Progress in the Development of a Kinetic Database for Heptane Combustion**," 41<sup>st</sup> American Institute of Aeronautics and Astronautic and Astronautics Conference & Exhibition, Reno, NV, January 7, 2003.
- Tsang, W., "**Multichannel Decomposition of Heptyl Radicals, 3<sup>rd</sup> Joint Meeting of the US Section of the Combustion Institute**," Combustion Fundamentals and Applications, University of Illinois at Chicago, March 15, 2003.
- Tsang, W., "**Kinetics of the Combustion of Real Fuels**," Combustion Research Facility, Livermore CA, May 23, 2003. Invited.
- Tsang, W., "**Progress Report - Database for soot formation in heptane combustion**," Wright-Patterson Air Force Base, May 25, 2003.
- Tsang, W., "**The Simulation of Real Combustion Processes**," Physical and Chemical Properties Division, NIST, MD, March 27, 2003.
- Tsang, W., "**Kinetic Data Base for Combustion Modeling**," 23rd Contractors Meeting Granlibakken, CA, May 28, 2003.



Tsang, W., "*Combustion Simulation Databases of Real Transportation Fuel*," Workshop on the Simulation of the Combustion of Real Fuels, NIST, Gaithersburg, MD, September 4, 2003.

### 3. Cooperative Research and Development Agreements (CRADAs) and Consortia

Development of Pulse Tube Refrigeration Technology for a Fully Acoustic Densifier that Simultaneously Conditions Two Cryogenic Fluids, R. Radebaugh  
**Sierra Lobo (CN-1744) (CRADA)**

Development of a Two-Stage Pulse Tube Cryocooler for Superconducting Motors, R. Radebaugh  
**American Superconductor Corporation (CN-1762) (CRADA)**

Development of a Pulse Tube Cryocooler for Dermatologic Cryosurgery  
**CIMEX BioTech (CN-1808) (CRADA)**

Praxair Pulse Tube Liquefier, R. Radebaugh  
**Praxair, Inc. (CN 1677) (CRADA)**

Coblentz Society/NIST Digitized Vibrational Spectra Database, S. Stein  
**The Coblentz Society (CRADA)**

Library Search Identification of Chemical Structure and Substructures from MS/MS Spectra, S. Stein  
**Finnigan Corporation (CRADA)**

North American Membrane Society Consortium: Pore Size Characterization Methodology and Standards for Ultrafiltration Membranes, C. Muzny  
**Merck, Millipore, Osmonics, Sartorius, Bureau of Reclamation**

Thermodynamics Research Center Research Consortium  
**Shell Development Company, Conoco Phillips, Chevron Texaco, Eastman Chemical Company, Virtual Materials Group, Inc.**

### 4. Patents

Bruno, T.J. and Rybowskiak, M.C., "Method and Apparatus for Entrainment Mixing of Vapor Into Liquids," U.S. Patent Number 6,585,405 (7/11/03).

Dobak, J., Radebaugh, R., Marquardt, E., and Huber, M.L., "Miniature Mixed Gas Refrigeration System," NIST #95-041PCT, International Patent Application.

Dobak, J., Radebaugh, R., Marquardt, E., and Huber, M.L., "Mixed Gas Refrigeration Method," NIST #96-040CIP-EPO, International Patent Application.

## 5. SRM Activities

SRM 217d 2,2,5 – Trimethylpentane (Iso-octane), Renewal, In progress, Certificate in 2003

Thermal Analysis Suite

SRM 2235 Bismuth, New, In Progress, Certificate in 2003

SRM 2236 Silver Bromide, New, In Progress, Certificate in 2003

Fluid Density Over Wide Ranges of Temperature and Pressure, New SD Project

Macropore Size Distribution Standard Disk (Membrane), New SD Project

## 6. SRD Activities

SRD NIST Chemical Kinetics Mechanism Database CKMech <http://srdata.nist.gov/ckmech/>

SRD 1/1ANIST/EPA/NIH Mass Spectral Library (Update: July 2002)

SRD 4 NIST Thermophysical Properties of Hydrocarbon Mixtures Database, Major Upgrade (Version 3.01), Support

SRD 10 NIST Thermophysical Properties of Water Database, Support

SRD 12 NIST Thermophysical Properties of Pure Fluids Database (Version 5.0), Support

SRD 14 NIST Mixture Property Database, Upgrade in Progress

SRD 17 NIST Chemical Kinetics Database on the Web, Version 7.0, Release 1.1

SRD 23 NIST Reference Fluid Thermodynamic and Transport Properties, Major Upgrade (Version 7), Support

SRD 23 NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures Database, Major Upgrade (Version 7.0), Support

SRD 40 NDRL/NIST Solution Kinetics Database on the Web, New Release

SRD 69 NIST Chemistry Webbook, Contributions on Fluid Properties, New Release

TRC Tables – Hydrocarbons, Major Upgrades

TRC Tables – Non-Hydrocarbons, Major Upgrades

International Data Series, Major Upgrades

SRD 85 NIST/TRC Table Database, WinTable 1.5 (2001), New Release

SRD 87 NIST/TRC Vapor Pressure Database, Version 2001, New Release

SRD 88 NIST/TRC Ideal Gas Database, New Release

## 7. Calibrations

Pratt and Whitney

Hoffer Flow Controls, Inc.

## 8. Committee Assignments

### **T.C. Allison**

Collaboratory for Multi-Scale Chemical Sciences

### **D.G. Archer**

ASTM Committee E37 on Thermal Measurements (Membership Secretary)

ASTM Subcommittee E37.02, Standard Reference Materials for Thermal Measurements (Chair)

ASTM Subcommittee E37.90, Executive Subcommittee (Member)

ASTM Taskgroup E37.01.06 on Heat Capacity (Chair)

ASTM Taskgroup E37.01.17 on Differential Scanning Calorimetry Calibration (Chair)

ASTM Taskgroup E37.01.21 on Reaction Calorimetry (Chair)

**P.E. Bradley**

NASA Cryogenic Technology Working Group for Space Exploration and Transportation

**T.J. Bruno**

International Forum on Process Analytical Chemistry, Scientific Board

ASTM Committee D03 on Gaseous Fuels

Gas Research Institute PCB Task Force

Annual SFE-SFC International Symposium, Technical Board

National Materials Advisory Board Panel on Separation Technology for Industrial Recycling and Reuse

**A.M. Chaka**

Secretary, Theoretical Subdivision, American Chemical Society

Member, Executive Committee, Physical Division, American Chemical Society

Secretary, Computational Molecular Science and Engineering Forum, American Institute of Chemical Engineers

**R.D. Chirico**

ASTM Committee E27 on Hazard Potential of Chemicals

**D.G. Friend**

ASME K-7 Standing Committee on Thermophysical Properties

ASME Research and Technology Committee on Water and Steam in Thermal Systems

ASME Subcommittee on Properties of Water and Steam

IAPWS Working Group on Thermophysical Properties of Water and Steam (Chair)

IAPWS Task Group on Transport Properties (Chair)

AIChE Design Institute for Physical Property Data (DIPPR): Project 991 Steering Team, Project 801 Steering Team, Administrative Committee, Technical Committee

Fourteenth International Conference on the Properties of Water and Steam Organizing Committee (Member)

Fifteenth Symposium on Thermophysical Properties (Organizer and Co-Chair)

Joint Conference of the 16<sup>th</sup> STP and ICCT 19, Executive Board (Vice President)

Industrial Fluids Simulation Challenge Organizing Committee (Member)

Industrial Fluids Simulation Challenge Benchmark Committee (Chair)

Joint ASME-AIChE Committee on Thermophysical Properties (Member)

**M. Frenkel**

Physical Data and Reaction Kinetics Committee (PDRK) of the Engineering Sciences Data Unit (ESDU<sup>TM</sup>), London, UK (Corresponding Member)

Committee for Data File Format Standardization of CODATA (IUCOSPED) (Member)

Board of Directors of International Association of Chemical Thermodynamics

Chair, Organizing Committee of ICCT-2006

Chairman, IUPAC Task Group

**A.H. Harvey**

ASME Research and Technology Committee on Water and Steam in Thermal Systems

ASME Research Subcommittee on the Properties of Water and Steam (Chair)

Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair).

IAPWS Working Group on Thermophysical Properties of Water and Steam

IAPWS Task Group on Fundamental Constants (Chair)

IAPWS Editorial Committee (Chair)

**R.E. Huie**

TSCA Interagency Testing Committee

NASA Panel for Data Evaluation

Titular Member, IUPAC Commission on Chemical Kinetics

## IUPAC Task Group on Standard Potentials of Radicals

### **A. Laesecke**

Colloquium Organizing Committee, CSTL, Boulder, CO (Co-Chair).

Board of Directors of the SURF NIST Boulder program.

IUPAC Project on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Organic Compounds and Mixtures (Coordinator) jointly with Prof. John Dymond (Glasgow, UK), Prof. Ulrich K. Deiters (Cologne, Germany), and Prof. Andreas Heintz (Rostock, Germany).

International Association of Transport Properties.

### **E.W. Lemmon**

Transmission Measurement Committee of the American Gas Association (AGA)

### **P.J. Linstrom**

ASTM Subcommittee E13.15, Analytical Data

### **J.W. Magee**

IUPAC Project on Thermodynamics of Ionic Liquids, Ionic Liquid Mixtures, and the Development of Standardized Systems (Coordinator)

IUPAC Project on Ionic Liquids Database (Coordinator)

Executive Board, 16<sup>th</sup> Symposium on Thermophysical Properties/19<sup>th</sup> IUPAC Conference on Chemical Thermodynamics

### **W.G. Mallard**

Steering Committee for the NIST/EPA/NIH Mass Spectra Database

Joint Committee on Atomic and Molecular Physical Data

Organization for the Prohibition of Chemical Weapons, Advisory Panel on the Central Analytical Database

### **M.O. McLinden**

ASHRAE Technical Committee 3.1 - Refrigerants and Secondary Coolants (Corresponding Member)

ISO TC86/SC8/WG7 – Refrigerant Properties (Member)

### **P. Neta**

Member, IUPAC Committee on Standard Potentials of Radicals

### **V.L. Orkin**

NASA Panel for Data Evaluation

### **R.A. Perkins**

ASTM Committee D34 on Waste Management

International Association for Transport Properties

### **R. Radebaugh**

International Cryocooler Conference, Inc., Advisory Committee

Cryogenic Society of America, Editorial Committee

### **J.L. Scott**

Measurement Technical Committee (MTC) for the GTI Metering Research Facility (MRF) at Southwest Research Institute (SwRI)

Transmission Measurement Committee of the American Gas Association (AGA)

### **S.E. Stein**

ASMS Subcommittee on Measurements and Standards – Methodology

IUPAC Committee on Printed and Electronic Publishing

IUPAC, The IUPAC Chemical Identifier (Project Leader)  
IUPAC, Standard XML Data Dictionaries for Chemistry (Project Leader)

## 9. Editorships

### **T.J. Bruno**

Journal of Process Analytical Chemistry (Associate Editor)

### **R.D. Chirico**

Journal of Chemical Thermodynamics (Editorial Board)

TRC Tables – Hydrocarbons (Editorial Board)

TRC Tables – Non-Hydrocarbons (Editorial Board)

### **M. Frenkel**

TRC Tables – Hydrocarbons (Editor-in-Chief)

TRC Tables – Non-Hydrocarbons (Editor-in-Chief)

International Data Series (Executive Director)

Computers and Applied Chemistry (China) (Editorial Board)

Vapor-Liquid Equilibria (Poland) (Editorial Board)

### **D.G. Friend**

International Journal of Thermophysics (Associate Editor)

TRC Tables – Hydrocarbons (Editorial Board)

TRC Tables – Non-Hydrocarbons (Editorial Board)

### **R.E. Huie**

International Journal of Chemical Kinetics (Associate Editor)

### **A. Laesecke**

Journal of Chemical and Engineering Data (Advisory Board)

TRC Tables – Hydrocarbons (Editorial Board)

TRC Tables – Non-Hydrocarbons (Editorial Board)

Guest Editor of a Special Issue of “Fluid Phase Equilibria” (Vol. 210, No. 1) with contributions to the 3<sup>rd</sup> IUPAC Workshop on Thermochemical, Thermodynamic, and Transport Properties of Halogenated Hydrocarbons and Mixtures, July 28-August 2, 2002, Rostock, Germany. (Invited)

### **J.A. Manion**

International Journal of Chemical Kinetics (Associate Editor)

### **J.W. Magee**

Journal of Chemical and Engineering Data (Associate Editor)

TRC Tables – Hydrocarbons (Editorial Board)

TRC Tables – Non-Hydrocarbons (Editorial Board)

### **P. Neta**

Radiation Physics and Chemistry (Editor)

### **R. Perkins**

TRC Tables – Hydrocarbons (Editorial Board)

TRC Tables – Non-Hydrocarbons (Editorial Board)

**R. Radebaugh**

Cryogenics (International Advisory Editor)  
Advances in Cryogenic Engineering (Editorial Board)

**J.C. Rainwater**

International DATA Series, Selected Data on Mixtures (Editor)

**W. Tsang**

International Journal of Chemical Kinetics (Editor)

**10. Seminars****October 30, 2002**

Jürgen Gmehling, Carl von Ossietzky University, Oldenburg (Germany), "Potential of Group Contribution Methods for the Prediction of Phase Equilibria and Excess Properties of Complex Mixtures" and "Online Demonstration of the Dortmund Database (DDB)." (Division Sponsor: A. Laesecke and W.M. Haynes)

**November 15, 2002**

Anthony R. H. Goodwin, Schlumberger-Doll Research, Ridgefield, Connecticut, "Micro Electro Mechanical System (MEMS) for the Measurement of Density and Viscosity." (Division Sponsor: W.M. Haynes)

**December 2, 2002**

Nordstrom, U.S. Geological Survey, Boulder, Colorado, "Application of Geochemical Model and Their Dependence on Reliable D. Kirk Thermodynamic Data." (Division Sponsor: W.M. Haynes)

**December 13, 2002**

J. Boerio-Goates, Brigham Young University, Provo, Utah, "Pure SiO<sub>2</sub> Zeolites -- Crystalline Materials with some Glassy Characteristics." (Division Sponsor: R.D. Chirico and M. Frenkel)

**December 20, 2002**

Ercang Luo, Chinese Academy of Sciences, Beijing (P. R. China), "Properties of Gas Mixtures and Their Use in Mixed-refrigerant Joule-Thomson Refrigerators at TIPC/CAS." (Division Sponsor: R. Radebaugh)

**February 14, 2003**

M. A. Anisimov, University of Maryland, College Park, Maryland, "Competition of Mesoscales in Near-Critical Polymer Solutions." (Division Sponsor: D.G. Friend)

**February 24, 2003**

D. Lary, NASA Goddard Space Flight Center, Greenbelt, MD, "Chemical Data Assimilation." (Division Sponsor: T.C. Allison)

**March 7, 2003**

T. Atake, Tokyo Institute of Technology (Japan), "Heat Capacity Measurements and Thermodynamic Studies of Molecular Motion and Phase Transition in Solids." (Division Sponsor: M. Frenkel)

**April 4, 2003**

V. Anikeev, Boreskov Institute of Catalysis, Novosibirsk, Russia, "Decomposition and Oxidation of Aliphatic Nitro Compounds in Supercritical Water" or "Modelling Density Effect on the Rate Constant of 2-Propanol Dehydration Reaction in Scw." (Division Sponsor: R.E. Huie)

**April 4, 2003**

L. Sun, Colorado School of Mines, Golden, Colorado, "Multiparameter Crossover Equation of State: Algorithm and Applications." (Division Sponsor: A.H. Harvey)

**May 5, 2003**

Jörg Baranski, Dept. of Chemistry, University Rostock (Germany), "Determination of Binary Diffusion Coefficients of Gases Using Holographic Interferometry in a Loschmidt Cell." (Division Sponsor: A. Laesecke)

**May 28, 2003**

R. Gomperts, Silicon Graphics, Hudson, MA, "Presentation on Gaussian 2003 and SGI Computers." (Division Sponsor: T.C. Allison)

**July 17, 2003**

M. Gordon, Department of Chemistry, Iowa State University, Ames, Iowa, "New Developments for Modeling Liquids and Solvent Effects." (Division Sponsor: K.K. Irikura)

**July 18, 2003**

R.J. Wheatley, University of Nottingham (England), "Calculating Intermolecular Potentials with SIMPER." (Division Sponsor: A.H. Harvey)

**August 18, 2003**

L. Greer, National Center for Biotechnology Information, National Institutes of Health, Bethesda, MD, "OMSSA: An MS/MS Search Algorithm for High-Throughput Proteomics." (Division Sponsor: S.E. Stein)

**August 28, 2003**

J. Dec, Sandia National Laboratories, Livermore, CA, "An Overview of Recent Research and Chemical-Kinetic Modeling needs for Internal Combustion Engines." (Division Sponsor: W. Tsang)

**11. Conferences/Workshops/Sessions Sponsored/Co-Sponsored**

Workshop on Combustion Simulation Databases for Real Transportation Fuels (R.E. Huie, J.W. Hudgens, J.A. Manion and W. Tsang, organizing committee).

Working Group Meeting on a Web Site for IUPAC/NIST Recommended Values for Thermodynamics, May 15 & 16, 2003 (R.E. Huie, J.W. Hudgens, J.A. Manion and T.G. Allison)

Symposium on Integrating Diverse Computational Approaches to Complex Problems, American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. A.M. Chaka and A.K. Wilson (U. North Texas), organizers.

15<sup>th</sup> Symposium on Thermophysical Properties, June 22-27, 2003, Boulder, CO (D.G. Friend)

**12. Other****T.J. Bruno**

Adjunct Professor, Department of Chemical and Petroleum Refining Engineering, Colorado School of Mines, Golden, CO.

**J.W. Magee**

Adjunct Professor, Department of Mechanical Engineering, University of Colorado, Boulder, CO.

**J.C. Rainwater**

Lecturer, Department of Physics, University of Colorado, Boulder, CO.

Ph.D. Advisor (S.A. Kadlec), Department of Physics, University of Colorado, Boulder, CO.

Foundations of Molecular Modeling and Simulation Conference, Keystone, CO. July 7-10, 2003. A.M. Chaka, organizing committee, NIST co-sponsored.

First Industrial Fluid Simulation Challenge Symposium, American Institute of Chemical Engineers Annual Meeting, Indianapolis, IN, November 3, 2002. R.D. Mountain, Case, F. (Colgate-Palmolive), Chaka, A.M., Friend, D.G., Frurip, D.(Dow), Johnson, R.D., Golab, J.(BP), Kolar, P.(Mitsubishi Chemical), Moore, J. (Dow), Schiller, M.(Dupont), and Storer, J.,