NBSIR 85-3039

Center for Chemical Engineering Technical Activities: Fiscal Year 1985

February 1986

National Engineering Laboratory
National Bureau of Standards
U.S. Department of Commerce
Boulder, Colorado 80303

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J. Hord, Editor

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National Research Council (NRC)
Board on Assessment of NBS Programs
February 26-27, 1986
Gaithersburg, Maryland

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Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1985 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science. They embody: development and improvement of measurement principles, measurement standards, and calibration services such as volumetric and mass flow rates, liquid volume, liquid density, and humidity; generation (via accurate measurement and advanced predictive models) of reliable reference data for thermophysical properties of pure fluids, fluid mixtures, and solids of vital interest to industry; and development of improved correlations, models, and measurement techniques for complex flows, heat and mass transport, mixing, and chemically reacting flows of interest in modern unit operations.

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INTRODUCTION

This document summarizes technical research activities of the Center for Chemical Engineering during Fiscal Year 1985 (October 1, 1984 through September 30, 1985). This Center is one of six such units that compose the National Engineering Laboratory of the National Bureau of Standards. A brief summary of the structure and technical activities of the National Bureau of Standards is given in the introduction portion of this report, along with organizational information on the Center for Chemical Engineering.

The activities of the Center are focused on chemical engineering in support of the chemical and related industries (including chemical, petrochemical, petroleum, gas, paper, biochemical, energy, food and drug, etc.). The goal of the Center is to provide the fundamental scientific framework for reliable measurement and data bases that assure equity in domestic and international trade; and enable improved innovation, design, and control of chemical processes. The Center's research contributes significantly to the ability of U.S. industry to compete in world markets.

This summary report is presented in three sections, one for each participating division in the Center: Chemical Engineering Science, Thermophysics, and Chemical Process Metrology. Each division summary is related in the same format but with individual style and emphasis. These summaries lead off with an introduction; state the division goal; outline division subelement (group) functions; summarize project activities; highlight major honors and awards of division staff; cite primary publications, talks,committee memberships, editorships, and professional interactions; and close with lists of conferences, workshops, and seminars hosted, sponsored, or organized by the division or Center.

An itemized table of contents is provided for the reader's convenience in locating specific technical topics of interest. If additional information is desired on any technical project reported herein, readers should address their inquiries to the appropriately identified project staff (and division) via the Center for Chemical Engineering, National Bureau of Standards, 325 Broadway, Boulder, CO 80303.

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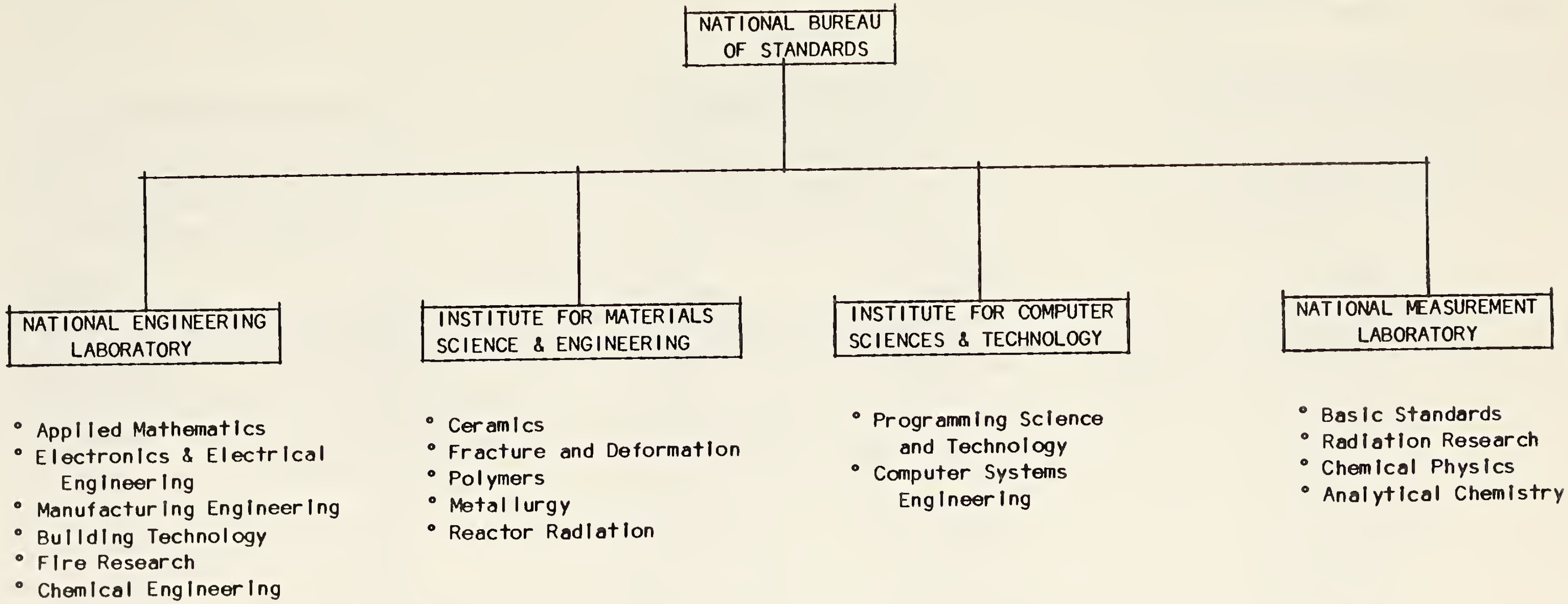

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- Unit Operations/Processes
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- Properties of Fluids
  (H. Hanley)
- Properties of Solids
  (L. Sparks)

Thermophysics Division
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- Statistical Physics
  (J. Kincaid)
- Equation of State
  (J. Levelt Sengers)

Chemical Process Metrology Division
J. Ulbrecht, Chief

- Flow Metrology
  (G. Mattingly)
- Multiphase Reacting Flows
  (G. Kulin, Acting)
- High Temperature Reacting Flows
  (H. Semerjian)
- Process Sensing
  (S. Hasegawa, Acting)

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Chemical Engineering Science Division (773)

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Properties of Fluids

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K. Bowie, Secretary

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Properties of Solids

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@D. Smith
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E. Buxton
D. Mann

* COOP - Cooperative Student Program
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@ Intermittent
\# National Research Council Postdoctoral Fellow
§ National Engineering Laboratory Fellow
° Guest Worker
°° Q-Appointment
† Industrial Research Associate
†† Full Time Temporary

Thermophysics Division (774)

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K. Heilers, Secretary
L. Phillips, Clerk Typist

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°P. Basu

Interfacial Phenomena - M. Moldover (Leader)
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*H. Chaar
°T. Edwards
J. Schmidt
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Dynamic Measurements - A. Cezairliyan (Leader)
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Statistical Physics

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°S. Lee
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***R. MacDonald
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*F. Martinez
°L. Rasaiah
@J. Sengers
D. Tsai

Equation of State

J. Levelt Sengers, Group Leader

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R. Chang
E. Clark
H. Davis
°F. Guzman
°D. Linsky
°°J. Manley
G. Morrison
#G. Nielson
°I. Pegg
°B. Taggart
°H. Woolley

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J. Mercer
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* COOP - Cooperative Student Program
** University Faculty Appointment (Intermittent)
*** Part Time
@ Intermittent
\# National Research Council Postdoctoral Fellow
§ National Engineering Laboratory Fellow
° Guest Worker
°° Q-Appointment
† Industrial Research Associate
†† Full Time Temporary
††† H. Raveche resigned this position, June '85.

Chemical Process Metrology Division (775)

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J. Whetstone
S. Arneson, Secretary (00)
S. Johnson, Secretary (01/02)
C. Mueller, Secretary (03/04)

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J. Hall	J. Houser	°°T. Ghazarian	K. Kreider
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N. Mease	***E. Moore	**A. Gupta	G. Scace
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		°°R. Schaerfl	
		°°D. Shaw	
		B. Shomaker	

Services Contracted
A. Humphrey
P. Klebanoff
J. Phillips

* COOP - Cooperative Student Program
** University Faculty Appointment (Intermittent)
*** Part Time
@ Intermittent
# National Research Council Postdoctoral Fellow
§ National Engineering Laboratory Fellow
° Guest Worker
°° Q-Appointment
† Industrial Research Associate
†† Full Time Temporary

MISSION OF THE NATIONAL BUREAU OF STANDARDS (NBS)

The basic mission of the National Bureau of Standards is to provide for the Nation's measurements and standards needs. NBS applies its expertise in science and engineering to foster the attainment of such national goals as: economic growth through innovation and productivity growth in industry and commerce, and through optimal utilization of labor, energy and material resources; reasonable and equitable regulatory decision-making with maximum benefit and minimum economic impact and uncertainty; equity in U.S. commerce through mutual understanding and acceptance of recognized transfer standards; and accuracy and compatibility in scientific communications and technology transfer among industry, government and academia, including the ability to make meaningful comparisons between the theoretical predictions and empirical data used in developing scientific knowledge.

Through performance of the functions set forth in the NBS Organic Act of 1901 and fourteen other statutes, the Bureau pursues its mission by fulfilling three major roles. The Bureau of Standards: (1) is the Nation's central reference laboratory and lead agency for the development and provision of measurement standards, measurement methods and techniques, and standard reference materials and data essential for the resolution of Federal, State, and local scientific and technical measurement issues; (2) addresses technological problems for the Nation through the application of basic physical, chemical, mathematical, and engineering science by providing traceability of measurements to national standards essential for ensuring measurement comparability, by uniform determination of the physical, chemical, and engineering properties of matter, and by provision of uniform methods for measuring the performance of materials, products, and engineered systems products; and (3) enhances the technological and scientific base of the Nation's productive sectors by developing basic technologies and information that underlie product and process development and innovation.

As a major operational unit of the Department of Commerce, NBS also contributes significantly to fulfilling the Department's mission to promote trade and commerce and to ensure the smooth and orderly working of our economy.

NATIONAL MEASUREMENT LABORATORY: Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes standard reference materials; provides standard reference data; provides calibration services; and collaborates with the Bureau's major organizational units in carrying out its responsibilities.

INSTITUTE FOR COMPUTER SCIENCES AND TECHNOLOGY: Provides scientific and technical services to the central management agencies (e.g., the Office of Management and Budget [OMB] and the General Services Administration [GSA]) to support the formulation of Federal ADP policies, the selection and direction of Federally sponsored computer research and development, and the resolution of policy issues affecting computer utilization; develops and recommends Federal Information Processing Standards; participates in the development of voluntary industry ADP standards in both national and international organizations; conducts research in the science and technologies of automatic data processing, computers, and networks; provides direct technical assistance to other Federal agencies in solving specific computer applications problems; cooperates with private sector users in determining standards requirements; cooperates with users in industry to test standards and develop certification techniques; conducts information exchange activities in the areas of computer and networking technologies; provides technical leadership for the development of national and international standards for ADP products in order to enhance the international trade position of the U.S. computer industry and to ensure that international standards do not form trade barriers; cooperates with representatives of foreign governments and organizations in research and testing activities; and monitors Federal Government participation in voluntary commercial standards development efforts.

INSTITUTE FOR MATERIALS SCIENCE AND ENGINEERING: Develops and maintains the scientific competences and experimental facilities necessary to provide the Nation with a central basis for uniform physical measurements, measurement methodology, and measurement services fundamental to the processing, characterization, properties and performance of materials, and to other essential areas in materials science; provides government, industry, universities, and consumers with standards, measurement methods, data, and quantitative understanding concerning metals, polymers, ceramics, composites, and glasses; characterizes the structure of materials, chemical reactions, and physical properties which lead to the safest, most efficient uses of materials, improve materials technologies, provide the bases for advanced material technologies in basic and high-technology industries, and encourage recycling; obtains accurate experimental data on behavior and properties of materials under service conditions to assure effective use of raw and manufactured materials, provides technical information such as reference data, materials measurement methods, and standards to processors, designers, and users for selection of cost-effective combinations of materials, processes, designs, and service conditions; uses the unique NBS reactor facilities to develop neutron measurement methodology, develop sophisticated structure characterization techniques, reference data, and standards; participates in collaborative efforts with other NBS organizational units in the interdisciplinary developments in materials science; and disseminates generic technical information from the Divisions to private and public sector scientific organizations through special cooperative institutional arrangements and through conventional distribution mechanisms.

NATIONAL ENGINEERING LABORATORY: Provides technology and technical services to users in the public and private sectors to address national needs and to solve national problems in the public interest; conducts research in engineering and applied science in support of objectives in these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; develops and improves mechanisms to transfer results of its research to the ultimate user; develops and demonstrates new institutional practices to stimulate use of technology; and collaborates with the National Measurement Laboratory in conducting its assigned responsibilities.

CENTER FOR CHEMICAL ENGINEERING: Performs research in process metrology, thermophysical properties of fluids and solids, and unit operations and processes; provides measurement practices and standards, fundamental engineering data, calibration and measurement services, and engineering science for the chemical process industry, academe, and Government.

CHEMICAL ENGINEERING SCIENCE DIVISION: Develops and maintains competence to provide essential engineering measurement and data bases that underlie the design and performance of chemical engineering processes and the behavior of solid materials of importance to the chemical and related industries; performs basic and applied research in unit operations (heat and mass transfer, and separations including membranes, chemical complexation, crystallization, selective adsorption, and liquid-liquid extraction), systems engineering, thermodynamic analyses of subprocesses, and scale-up; performs thermal and related properties measurements research to develop data-predictive models and reference materials for solid feedstocks and fuels (coal and gas hydrates) and for technical solids (insulating materials, metals, alloys, polymers, composites, and ceramics); provides critically evaluated data, measurement standards, predictive models, and engineering correlations in these research activities.

THERMOPHYSICS DIVISION: Develops new measurement techniques, thermodynamic models, and molecular theories to describe the thermophysical behavior of condensed matter ranging from classical fluids and solids to highly complex fluid mixtures containing molecules of varying size, polarity, and chemical nature. Research includes multicomponent-multiphase fluid mixtures, interfacial phase transitions, nucleation, computer simulation of fluid behavior, critical point phenomena and properties, properties of supercritical fluids, phase separation, equations of state, and transport processes in fluids and high-melting temperature metals. Results include: theoretically-based predictive models and correlations that use transportable computer codes to predict thermophysical properties of condensed substances; state-of-the-art experimental measurements; and critically evaluated properties data.

CHEMICAL PROCESS METROLOGY DIVISION: Develops improved measurement techniques, theoretical and computational models to describe and qualify the performance of laboratory and process plant instruments, and complementary advanced fluid dynamics analyses/models to explain the behavior of fundamental fluid flows; develops experimental and theoretical means to characterize fluid behavior (solid-fluid slurry flow modes, fluidized beds, chemically reacting flows, etc.) and to evaluate the performance of combusting flows (gaseous, liquid, solid and slurry fuels) with emphasis on high temperature, corrosive and erosive exhaust streams; develops measurement standards and provides measurement services for flow (volume and mass rates), fluid density, fluid volume, and humidity; and provides advanced measurement techniques, standard measurement practices, and technical data (experimental, theory and computer models) for measurement, analysis and control of chemical processes.

TECHNICAL ACTIVITIES
OF THE
CHEMICAL ENGINEERING SCIENCE DIVISION (773)

M.J. Hiza, Acting Chief

1. INTRODUCTION

The ability to accurately model processes has long been important to the efficient design and operation of the plants and facilities in the chemical, petrochemical, petroleum, gas, and related industries. The rising cost of energy during the past decade has sharpened this need. In like manner, these industrial processes are steadily moving toward alternative and much more complex base feedstocks which in turn yield more complex, and often, corrosive and hazardous conversion products. In order to accurately model processes in conventional and the newer and more unconventional plants, one needs a reliable and well documented data base for the properties involved as well as accurate models for the unit operations represented within these industrial processes. The work of the Chemical Engineering Science Division is focused on providing the measurements and data needed for the properties involved and on advancing the state-of-the-art for unit operations. The key ingredients are measurements, measurement standards, benchmark data, and theoretically based predictive models for properties of solids and fluids and for engineering systems. In addition to contributions related to process design and operation, the work of the Division is heavily involved in measurements and data necessary for accurate and verifiable custody transfer of chemicals and fuels.

In all areas that relate to the research of the Gaithersburg Divisions, close collaborative interactions have been developed. There is close collaboration with the Thermophysics Division with complete integration of the fluid and solid properties efforts, and with the Chemical Process Metrology Division in flow research. These collaborations include several joint projects sponsored by other agencies, and new ones are being initiated.

One of the primary focuses of research in the Division is related to new base feedstocks. For the most part a thorough and quantitative understanding of the behavior of the molecular parameters and bulk properties of these new chemical systems does not presently exist. The complexity of the phenomena involved and the vast array of fluids and solids encountered precludes the possibility of a purely experimental or correlative approach. It is essential that the approach be one which carefully integrates experiment, theory, and evaluation so as to yield accurate property and unit operations predictive models, Standard Reference Data, and Standard Reference Materials which are as broadly applicable as possible. For these reasons, the theoretical effort will break new ground in molecular parameters, metastability, phase equilibria involving multiple phases, non-Newtonian fluid behavior and related nonlinear phenomena, interfacial phenomena, heat and mass transfer, and other unit operations. Similarly, new measurement procedures are being developed to handle corrosive and hazardous fluids, to perform measurements in regions heretofore inaccessible, and to provide measurements of higher accuracy or by simpler and more efficient means than currently available. This program addresses scientific issues of concern to industries which have made great strides in recent years in the use of process simulation and computer-aided design in the development and optimization of processes and plants. It is essential that the models and data resulting from this program be published in a form which can be readily incorporated into these modern computer-based tools.

The research of the Division addresses scientific issues of national interest in which NBS expertise and its impartial position are critical to an acceptable resolution, as with the highly accurate measurement and modeling of properties of fluids such as ethylene, the lower molar mass alkanes, and selected mixtures. The majority of the effort, however, is directed toward problems of the future. These include, but are not restricted to: 1) fluid and material properties and processes related to conversion of coal to gases and liquids such as synthesis gas, methanol, etc., for use as chemical feedstocks and fuels; 2) biomass derivatives as fuel and chemical feedstocks, e.g. alcohol systems; 3) the efficient use of heavy oils, tar sands, and other highly viscous fluids which exhibit nearly solid-like behavior; 4) the utilization of less energy intensive separation processes; and 5) properties of biosubstances and bioproduct separation/purification technology needed for large scale manufacture of biochemicals. The strategy is to perform basic research, generic to the science underlying the chemical, biochemical, and petrochemical processing industries, which requires the special role of NBS as an impartial national laboratory excelling in measurements and their interpretation. During the past year, the effort in membrane separations research has been modified somewhat, to accommodate new plans for a project on bioseparations. The transient heat transfer project was completed and new work was initiated on heat transfer in supercritical extraction processes. Plans have been developed to initiate new research projects on thermal properties of ceramics and polymer composites.

In addition, the Chemical Engineering Science Division serves other government agencies, industrial consortia, trade associations, etc., by providing research which is appropriate to the mission of the National Bureau of Standards and which is consistent with the goals of the Center for Chemical Engineering and the Division. This externally supported research constitutes a major part of the planned effort in achieving the goals of the Division.

2. GOAL

The goal of the Division is to provide evaluated engineering reference data; standard measurement procedures and test methods; predictive techniques, correlations, computer codes, and underlying theory needed by the chemical and related industries to innovate, design, and control chemical processes.

The output of this program assists these industries in maintaining and enhancing their competitiveness in the international marketplace. The primary means of accomplishing this goal is by providing theoretically based predictive techniques, critically evaluated data, and state-of-the-art measurement techniques. The approach is to conduct research on fundamental theoretical models, new concepts and phenomena, and predictive algorithms in synergism with experimental programs. This approach nurtures development of new measurement techniques, provides accurate data on unit operations, and on the properties of carefully selected pure fluids, mixtures, and solids which are representative of broad classes of substances. An essential corollary of these efforts is the critical evaluation and correlation of experimental data leading to the publication of Standard Reference Data, development of Standard Reference Materials, and development of voluntary-standard measurements and test methods.

3. GROUP FUNCTIONS

The research of the Division is organized into three technical groups: Unit Operations/Processes, Properties of Fluids, and Properties of Solids.

o Unit Operations/Processes - S.K. Sikdar, Group Leader

The Unit Operations Group performs experimental, theoretical, and mathematical modeling research in: separation of gases, solutions and biochemicals; heat transfer; flow measurement, including facilities for mass-based gas and cryogenic liquid flow; and process thermodynamics, the analysis of processes and techniques.

o Properties of Fluids - H.J.M. Hanley, Group Leader

The Fluid Properties Group has a research program which integrates experimental measurements, theoretical studies, and critical evaluation of data, all designed to lead to an understanding of fluid behavior. Outputs are data and theoretically-based predictive models for the properties of complex mixtures and technically important pure fluids. The fluids of interest are industrial chemicals, hydrocarbons, coal conversion products, heavy oils, biochemical solutions, etc.

o Properties of Solids - L.L. Sparks, Group Leader

The experimental and analytical research of the Solid Properties Group is focused on the thermal properties (thermal conductivity, thermal expansion, and heat capacity) of industrially important solids such as: solid fuels (e.g. coal and gas hydrates); and foams, fibers, fiberboards, aggregates, metals, ceramics, composites, and polymers. In addition, work is performed on the ignition and combustion characteristics of metal alloys, in an oxygen environment, at pressures up to 20 MPa.

4. SELECTED PROJECT SUMMARIES

UNIT OPERATIONS/PROCESSES GROUP

Separations Research - Measurements, Standards, and Modeling

R.D. Noble, J.D. Way, G.J. Hanna, R.A. Perkins, L.A. Powers, K.M. Larson, S.K. Sikdar

The objective of this research is to develop basic measurement techniques and standards, provide a body of high quality experimental data, and develop predictive models and computer codes for the use of chemical complexation in separation processes. The separation technique currently used in the research is facilitated transport in liquid membranes; however, reversible chemical complexation can be applied to liquid-liquid extraction, extractive distillation, absorption, and others. Measurements are made to study basic transport properties, acquire mass transfer data, and understand mechanisms. The fundamental models, developed using these data, can then be applied to any of the several processes using chemical complexation. The experimental work uses immobilized liquid membranes for gas phase studies and emulsion liquid membranes for liquid phase systems. Measurements involve CO, CO_2 and H_2S removal from gas streams, and removal of metal ions (such as copper) and organics (such as amines) from aqueous streams. A new thrust in bioprocessing has been initiated. This bioseparations research includes studies on the partition of proteins in two-phase aqueous extraction, separation of amino acids by ion-exchange membranes, and measurements of protein diffusivities in aqueous solutions. The major objective in these studies is to provide data and understanding necessary for design of industrial bioseparation processes. Externally funded work includes study of acid gas (CO_2 and H_2S) removal from natural gas streams for the U.S. Department of Energy, and research on removal of organics and heavy metals from aqueous streams for the U.S. Environmental Protection Agency.

Heat Transfer

V.D. Arp, P.J. Giarratano, W.G. Steward, M.C. Jones, S.D. Bischke, R.D. Nassimbene

The transient heat transfer project has been completed. This work combined theoretical studies with two types of experimental measurements. One experimental study involved investigation of the nonlinear interaction between a transient heat pulse and the resulting induced fluid flow in a long line.

The main output of this study is a new, general-purpose computer code valid for fluid mixtures as well as for pure fluids. The second study used optical techniques to study, quantitatively, the behavior of fluids immediately adjacent to a pulse heated surface in an open system. Data have been taken both in the laboratory and in near zero-gravity aboard a NASA KC-135 (to avoid buoyancy effects). Measurements support a heat transfer model based on thermally driven fluid motion, and at the same time defined a limit to the applicability of optical techniques under high temperature gradient conditions.

The heat transfer project has been redirected to study the problems of heat transfer in the retrograde condensation of a supercritical fluid mixture. The apparatus containing the supercritical test loop has been designed, fabricated and is in the process of being assembled for initial tests.

Metering of Natural Gas and Cryogenic Liquids

J.A. Brennan, B.R. Bateman, P.R. Ludtke, S.E. McManus, C.F. Sindt
J.D. Siegwarth, I. Vazquez, D.B. Mann

At the core of this work is a flow facility capable of providing accurate and precise mass-based data for flowing cryogenic liquids and ambient temperature gas. There are four projects currently under study. The first is aimed at providing substantial improvement in the metering of natural gas by means of orifice plates. This multi-year program, funded by the Gas Research Institute, includes an extensive series of measurements on a 4-inch diameter orifice meter used for interlaboratory comparisons in Europe. Also under investigation are swirl phenomena, flow conditioning concepts, and required straight pipe lengths. The work in Boulder on gas flow is closely coordinated with similar work on water flow in Division 775 (sponsored by the American Petroleum Institute). The second area of flow research utilizes the flow facility to evaluate new measurement techniques and to perform special tests on meters to provide measurement traceability to NBS. These tests are performed with liquid nitrogen. The third area of flow research is concerned with high velocity flows (over 50 m/s), and utilizes water from a local hydroplant since such velocities are well beyond the range available in a laboratory. The purpose of this work is to assist NASA in developing reliable flowmeters for the Space Shuttle Propulsion System. The last area of research is aimed at providing measurement manuals for natural gas and liquefied natural gas (LNG). One project, supported by an international consortium of gas importing firms and covering all aspects of custody transfer (including flow measurements), is nearing completion. Another project, completed with support from the USAF, dealt with natural gas metering, heat content measurement, and calculation of purchased energy.

Process Thermodynamics

V.D. Arp, D.E. Daney, M.J. Hiza, B. Louie, J.D. Siegwarth,
W.G. Steward, R.O. Voth

This work is designed to provide engineering, principally cryogenic engineering, expertise to other government agencies to solve a variety of problems. Current research is concerned with 1) performing experiments on condensed cryogens and evaluating the thermodynamics of, and heat and mass transfer effects in, systems used in inertial confinement fusion; and 2) analyzing the fluid mechanics and thermodynamics involved in the transfer and storage of large quantities of fluids such as liquid hydrogen, oxygen, and helium in low gravity environments, and the mixing of hydrogen and oxygen liquids. The work in area 1) is supported by the Department of Energy (DOE) and in area 2) by the National Aeronautics and Space Administration (NASA).

PROPERTIES OF FLUIDS GROUP

Integrated Study of Fluid Properties

H.J.M. Hanley

The fluid properties group has a strong background in experiment, theory, correlation, and data dissemination for the properties and behavior of fluids. Recently, the thrust has been to broaden the capability to more complex mixtures and to cover a wider temperature range. The approach is an integrated effort of experiment, correlation of data, and theory that is as fundamental and broadly based as possible. It is felt that a general approach is versatile, flexible, and in the long run, productive; specific objectives can then be met by the appropriate emphasis. Examples of our output would include data for supercritical extraction, the properties of synthetic gas and coal derived fluids, properties of hydrocarbons and chemicals (e.g., methanol, benzene, toluene), the production of design data for large scale CO_2 and N_2 custody transfer, industrial chemical processing, and data and models for advanced gas separation processes.

The experiments involve accurate measurements of selected pure components and binary mixtures, and multicomponent mixtures when appropriate. Theoretical studies are concerned with the basic properties and structure of fluids. Data evaluation and correlation facilitate coordination of the experimental and theoretical studies. Fluids are selected because of their industrial importance and to serve as models for wide classes of industrially important systems. For example, hydrogen sulfide, carbon dioxide, and carbon monoxide are important components of industrial mixtures in general, but are also typical of the class of inorganic polar molecules occurring in substitute feedstocks and coal derived liquids. Mixtures with organics, e.g., CO_2 +

butane are again of major industrial interest (such as in the problem of supercritical extraction), but are further representative of even more complex mixtures which invariably contain components of differing chemical nature, size, and/or polarity. An important final objective is to develop predictive procedures packaged as computer programs or other forms most appropriate for the user. This work is the core of the fluid property program and includes the basic NBS support, but in addition receives research funds from the Department of Energy (DOE)-Office of Basic Energy Sciences, the Gas Research Institute (GRI)-Basic Research, the NBS-Office of Standard Reference Data, and the National Aeronautics and Space Administration.

Supercritical Fluid Properties

J.F. Ely, J.W. Magee, J.R. Fox, W.M. Haynes, L.A. Weber, T.J. Bruno

Recent industrial interest in enhanced oil recovery with near critical carbon dioxide, supercritical fluid extraction, and near critical custody transfer of commercial chemicals has pointed out the need for accurate data and models for supercritical fluid mixtures. One project, which is supported by a consortium of 13 companies and an industrial trade organization, enables us to develop accurate predictive models for this type of fluid and accurate experimental data which can be used to test and further develop the predictive models.

Thus far, this project has produced: a comprehensive equation of state, based on the Wagner equation, for pure carbon dioxide; preliminary equations for selected refrigerants; a "state-of-the-art" computer code, useful for custody transfer of supercritical fluid mixtures, especially those rich in carbon dioxide; a general predictive model for fluid phase equilibria and bulk phase properties of mixtures; experimental PVT data for carbon dioxide from 220-330 K at pressures to 35 MPa; and phase equilibria data for binary mixtures of carbon dioxide with normal butane and isobutane from 250-394 K. Current experimental efforts are directed toward refrigerants; these include PVT data for R13 and R23 from 100 to 330 K at pressures to 35 MPa, and phase equilibria data for binary mixtures of normal butane, isobutane, R13, and R23 from 300 to 400 K.

A second project, supported by DoE-Office of Basic Energy Sciences, involves exploratory research on and evaluation of a supercritical fluid chromatograph. Carbon dioxide will be used as the carrier gas in a study of the diffusivities of fused ring polynucleararomatic hydrocarbons.

Viscosity and Thermal Conductivity Measurements

D.E. Diller, H.M. Roder

Measurements on viscosity and thermal conductivity are vital to complete the data base needed by the design engineer and are a necessary adjunct to PVT and thermodynamic properties. Further, the behavior of transport coefficients is very interesting from a scientific standpoint and demonstrates the fascinating and versatile behavior of a fluid in nonequilibrium. We have an ongoing program to measure the viscosities of dense fluids and mixtures, from 80-320 K, from the gas phase to the very dense liquid phase using a piezoelectric crystal viscometer. Recent results are available for mixtures of CO_2 + ethane, methane + ethane, and for CO_2, n-butane, and i-butane. Thermal conductivity data are taken with a transient hot wire apparatus over the same range. Recent results on the thermal conductivity of methane + ethane mixtures have unambiguously demonstrated that the mixture displays an enhancement in the critical region which contradicts theoretical predictions. The critical enhancement in mixtures appears very similar to the critical enhancement in pure fluids. Theory predicts enhancement in pure fluids, but strongly suggests that it should not be present in mixtures. The results of both transport property studies are the first accurate and comprehensive experimental data for mixtures.

A new high temperature viscometer is nearing completion and performance testing. It will cover the temperature range of 300-600 K with pressures to 35 MPa. The first measurement program will include heavy hydrocarbon systems. A new high temperature transient hot-wire thermal conductivity apparatus is also under construction and will operate at temperatures up to 650 C and at pressures up to 80 MPa. Again, the emphasis will be on fluid systems which are suitable for the development of predictive models for complex fluid mixtures of industrial importance.

Phase Equilibria Data for Industrial Fluids

J.E. Mayrath, L.A. Weber, T.J. Bruno

Phase equilibria (VLE, fugacity) studies are a major component of the group's effort. We have recently completed construction of a conventional circulation total pressure system designed for operation between 300-500 K. The systems CO_2 + n-butane, and CO_2 + i-butane have been studied. The object was to better understand the influence of the isomers in an organic + inorganic mixture. Current work includes binary mixtures of butanes and halogenated hydrocarbons. It should be noted that a similar low temperature VLE apparatus was also used for measurements on the CO_2 + butane systems. A high temperature VLE apparatus for operation from 300-900 K is available and being improved. The apparatus can operate in two modes. A mixture at constant composition and known total mass is pumped into a cell at a given temperature, and the pressure is measured for a given volume of the fluid in the cell. There are breaks in the pressure-volume curve as the fluid goes through the dew and bubble points. The concentration is changed and the procedure repeated. Hence a dew/bubble point curve is traced out. The system studied is methanol + water. The second mode is as follows: the components of the mixture are mixed at room temperature to give a mixture of known volume fraction. The feed mixture is pumped at constant flowrate (of the order of microliters/s) into a cell at the temperature (T) of interest where it will split into two or more phases at sufficiently high temperature. We have the freedom to set either the liquid (x) or vapor phase composition (y) to that of the feed by withdrawing samples of the chosen phase at the same mass flowrate as that of the feed. At a steady state, we thus know T and either x or y and measure the pressure. Differential refractometry is used to compare the composition of the feed to the material being withdrawn, with the flowrates adjusted to ensure equality. The composition of the excess phase is withdrawn at a flowrate two or three orders of magnitude less than the rate of the feed and its composition determined by differential refractometry with respect to the feed. By varying the original feed composition, one has a continuous calibration detection device. CO_2 + naphthalenic systems will be studied.

Another operational device is designed to study hydrogen mixtures. We have constructed a system with a palladium membrane through which pure hydrogen is in contact with a hydrogen mixture. By measuring the properties of the pure hydrogen we obtain the fugacity of hydrogen in the mixture. Results are available for H_2 + CH_4, H_2 + C_3H_8, and H_2 + CO_2 mixtures. H_2 + CO studies are nearly complete.

PVT Measurements of Industrial Fluids

G.C. Straty, W.M. Haynes, J.W. Magee

The group has three operational apparatus to measure the PVT properties of fluids: a direct density measurement magnetic densimeter based on Archimedes principle operating between 80 and 320 K for pressures to 35 MPa; an isochoric PVT cell operating under the same conditions; and a high temperature cell for 300-900 K with pressure to 50 MPa. The latter apparatus can handle toxic, explosive, and chemically reactive materials. Recent results include data for CO_2, CO_2 + N_2, H_2S, methanol, and benzene. The low temperature PVT cell is currently being automated for measurements on R13 and R23. We are also raising the upper temperature limit. The high temperature apparatus has been specifically designed for use with chemically reactive fluids and is currently being used for toluene measurements. Measurements are made along isochores with all data taken on a given isochore in an automated mode. An isochore will normally involve 18-20 measurements with 20-30 isochores measured for a given fluid.

Prediction of Fluid Properties

R.D. McCarty, R.D. Goodwin, J.F. Ely, D.G. Friend, J.C. Rainwater, M.R. Moldover, H.J.M. Hanley

A primary output of the group is the correlation of a set of data and/or a prediction procedure packaged for the user involved in science or engineering. Correlations for several pure fluids have been developed recently: H_2S, CO, CO_2, ethylene, methanol, for example. Prediction packages include TRAPP (transport property prediction procedure), MIPROPS (properties of eleven pure fluids), and SUPERTRAPP (phase equilibria, properties of mixtures) which is to be released soon. These procedures are the visible results of a basic study of fluid behavior and the application of statistical mechanics and kinetic theory.

We are studying methods to predict the properties of polar mixtures, and we are investigating VLE near the critical point and the prediction of critical lines for mixtures. The latter is directed toward development of a computer predictive package. We are also developing correlations in the form of computer packages for spacecraft propellants and life support fluids under the sponsorship of the NASA.

Fundamentals of Fluid Behavior: Equilibrium and Nonequilibrium

H.J.M. Hanley, J.C. Rainwater, J.F. Ely, D.G. Friend

A long-term investigation is under way to study the behavior and structure of fluids and their mixtures. We are especially interested in fluids of complex structure, e.g., polar molecules, and mixtures whose species are substantially different in physical or chemical nature. We are also interested in unusual conditions, e.g., when the fluid is at a state near a critical point or line, or close to freezing. In particular, nonequilibrium fluid behavior is a subject of considerable current concern. Basic theoretical questions arise on the definition and thermodynamic concepts once a fluid is not at equilibrium. Also, from the practical standpoint, the engineer needs transport properties and a knowledge of flow behavior in these thermodynamic regions for proper design and efficient operation of process equipment. We are undertaking a very general study of fluids subjected to a shear and a temperature gradient. We have shown that even the simplest fluid is basically non-Newtonian and that there is a definite relation between the equation of state of a fluid (and hence its thermodynamic properties) and the departure of the fluid from equilibrium. Specific recent outputs of the work include: mixing rules and local composition for mixtures of diverse species, effect of shear on phase equilibria of mixtures, and a priori calculation of the behavior of a fluid when stirred or mixed. Shear induced phase phenomena, with applications to suspensions, slurries, and multiphase flow are also under investigation. The direction of the work is a fundamental understanding of the nature of complexity. The results will then yield theoretical knowledge of mixtures which will in turn aid in the development of predictive techniques for broad classes of fluids.

Measurement of Thermodynamic Properties of Fluids

J.W. Magee, B.A. Younglove

There is an awareness in industry that data for the derived thermodynamic properties (e.g., specific heat, velocity of sound, enthalpy) of even simple fluids and mixtures are sparse. Further, the predictions of such properties from an equation of state are unreliable without data to check and optimize the forecasts. Isochoric specific heat data have been obtained for CO_2 from 220 to 330 K at pressures to 35 MPa. Current work includes initiation of measurements on the methane + ethane system. These results are of immediate relevance to the gas industry and for use in supercritical fluid processes. They are also used in development of theoretically based prediction procedures.

Sound speed measurements are under way on methane + ethane mixtures. These results will be used in the development of highly accurate sound speed correlations which will be used, in turn, for reducing the uncertainty in natural gas flow measurements using sonic nozzles.

Properties of Chemically Reacting Systems

T.J. Bruno, J.E. Mayrath, G.C. Straty

A new thrust of the group is to develop techniques to measure and report the properties of fluids that can react chemically (decompose). We have prepared a set of guidelines suggesting steps that experimentalists should follow to present the data in a useful and reproducible manner. We have undertaken the substantial task of setting up an analytical laboratory containing the equipment needed to analyze the composition of possible reacting fluids and reaction products. The equipment presently consists of a gas chromatograph, a liquid chromatograph, an ultraviolet spectrophotometer, and an infrared spectrophotometer. A mass selective detector and electron capture detector will be added soon. The entire laboratory is explosion proof and can handle toxic substances. We have already experienced the problems of reactive test fluids with our PVT measurements on H_2S, methanol, and benzene and phase equilibrium studies of methanol + water. Chemistry is also an integral part of our investigations of H_2 + organic systems in contact with a palladium membrane, and of our studies with a supercritical fluid chromatograph.

Association in Coal Liquids

A.J. Kidnay, J.F. Ely, H.J.M. Hanley, T.J. Bruno

Predictive procedures that are, in general, successful for relatively simple mixtures (such as the alkanes) can fail when applied to partially defined liquids such as coal liquids or petroleum fractions. The problem, however, is not necessarily a failure of the procedure per se, rather it can be the uncertainty in the input parameters (such as pseudocritical parameters). If the mixture is associated or hydrogen bonded, the difficulties are compounded and then the procedure may need modification. The engineer needs a simple check to see if a given liquid is associated or not, and then needs parameters to enter into the appropriate prediction procedure. Two experimental approaches have been selected in an attempt to quantify the problem of association in undefined liquids. These are measurements of viscosity and heats of mixing. Comparisons with predictive models, such as TRAPP, have demonstrated that viscosity measurements can serve as a screening test to distinguish between nonassociating and highly associating mixtures. Model coal liquids with known associating compounds were constructed for these investigations. Only preliminary studies have been done on heats of mixing. This experimental work is designed specifically to aid in the theoretical understanding of these complex systems.

PROPERTIES OF SOLIDS GROUP

Solid Fuels Research

J.E. Callanan, B.J. Filla, J.F. Hurley, J.G. Hust,
L.L. Sparks, S.A. Sullivan

The techniques developed for measurement of the heat capacity of raw coals are being extended to higher temperatures, to coals of different ranks, and to macerals, premium coals, and chars. Experimental efforts in the near future will be directed toward evaluation of the total enthalpy of an exothermal reaction which has been observed on the initial heating of raw coal. Through collaboration with other coal scientists we will attempt to understand this reaction. Other experimental results which will aid in reaching this understanding include: measurements on macerals to permit evaluation of the mineral contribution to the overall reaction; measurements on premium coals to allow for evaluation of the effects of oxidation; heat capacities measured in varied atmospheres (air, nitrogen, argon, helium, and carbon monoxide); heats of desorption measured by a newly developed technique; and analysis of effluent gases.

A series of coal-epoxy specimens, with different proportions of the two components, have been prepared for use in thermal conductivity measurements, with a compression probe, on powdered coal. These results will be compared with those from linear hot-wire measurements on powdered and chunk coal.

All experimental data generated are being used in a modeling program for thermal properties of coal under way in Division 774 of the Center. Agreement to date with a model for the carbonization of coal, proposed by Merrick of the Coal Research Establishment, U.K., has been excellent. However, extension of the measurements, and thus the modeling, to higher temperatures will allow us to examine a critical region for the thermal properties of coal, 600 K to 1000 K. The studies on rank series are in collaboration with Southern Illinois University.

A calorimetric technique for measuring the heat of desorption of water from porous solids was developed. It will be used to determine heats of desorption for other solid-liquid systems. A modification of the technique should allow calorimetric measurement of heats of adsorption in solid-gas systems.

Work on gas hydrates has continued with partial support from DoE, Morgantown. A cutting device that allows preparation of smooth surfaces suitable for use in thermal measurements has been constructed. Techniques for sample preparation have been developed which allow for preparation of uniform specimens under carefully controlled conditions, which can be repeated exactly. Specimens of two types of hydrates have been prepared and heat capacity measurements by an enthalpic technique are underway. The system for thermal expansion measurements has been altered to increase sensitivity and will be tested on ice before use with clathrates.

Development of SRM's

J.G. Hust, J.E. Callanan, S.A. Sullivan

Research has been directed toward the establishment of several thermal property Standard Reference Materials (SRM's).

The glass fiberboard SRM of thermal resistance (SRM 1450b) has been certified for temperatures from 100 to 330 K. This is an extension of the previous certification at temperatures from 255 to 330 K.

A new SRM for thermal resistance, glass fiberblanket, SRM 1451, has been established for the temperature range 100 to 330 K.

A proposal has been funded by DoE for the development of high-temperature insulation SRM's. These SRM's will fill an existing gap in the range of available thermal conductivity SRM's, and are of interest to researchers and manufacturers in the chemical process industry.

Zinc (SRM 2221) and tin (SRM 2220) have been certified as temperature and enthalpy-of-transition standards according to procedures outlined in NBS Special Publication 260-99. The certification program will continue with certification of standards for room temperature, subambient, and high temperature regions. The heat capacity of 9-methylcarbazole has been measured by adiabatic calorimetry from 6 to 345 K and by differential scanning calorimetry from 125 to 350 K. A comparison of these results will complete a feasibility study to determine whether heat capacity standards can be developed by scanning calorimetry.

Cryocooler Studies

R. Radebaugh, J. Zimmerman*, B. Louie

A pulse tube refrigerator was built under a NASA-Ames contract and reached a record low temperature of 60 K in one stage. The lowest temperature previously reached with a pulse tube refrigerator was 105 K by a group from Moscow Technical High School. This new work has led to the device becoming a serious alternative to other refrigeration schemes that have more moving parts. The pulse tube refrigerator has only one moving part. A test apparatus to measure the efficiency and refrigeration power per unit mass flow has been constructed under the same program. A paper on this new development was presented at the 1985 Cryogenic Engineering Conference.

Under a five-year Air Force contract, the regenerator test apparatus was modified to make tests in the presence of pressure waves to simulate the environment seen by regenerators in an actual refrigerator. A high specific-heat material, GdRh, has been formed into powder for testing as a regenerator. This material has been sent to Hughes Aircraft for tests in an actual refrigerator, after which precise effectiveness values will be determined over a wide range of conditions in our regenerator test apparatus. An important part of the regenerator test apparatus is the high speed thermometer to measure the instantaneous gas temperature on both sides of the regenerator. The silicon-on-sapphire thermometers, made at NBS and Stanford University, are the fastest responding thermometers in existence with a measured self-heating response time of 300 ns. A paper describing these thermometers has been written and is awaiting Air Force approval for publication.

The least reliable component of present cryocoolers is the mechanical compressor. A proposed alternative uses a thermal compressor in which the gas to be compressed is first adsorbed on charcoal at a low pressure. The charcoal is then heated slightly and the adsorbed gas is driven off at some higher pressure. Only slow-moving check valves are needed to provide continuous flow in one direction. The necessary data to design a helium-charcoal compressor is lacking, but a program funded by the Air Force Space Technology Center will enable us to measure the adsorption characteristics of helium on charcoal in the temperature range 10 to 77 K. The apparatus to make such measurements was completed in FY85.

*NBS Center for Electronics and Electrical Engineering

Metal Combustion in High Pressure Oxygen

J.W. Bransford

A program to study the ignition and combustion characteristics of a number of metals and alloys in high pressure oxygen, pressures to 20 MPa, has been undertaken for NASA. This program is not only of interest to NASA and the aerospace industry, but also to producers, transporters, and industrial users of liquid and gaseous oxygen.

The top surface of a cylindrical sample is heated by a focused CO_2 laser beam. Interior and exterior temperatures are measured before, during, and after ignition. Also measured is brightness (for correlation to previous work) and weight increase (for combustion rates). High-speed movies of the ignition and combustion process are also made.

From the above data, ignition temperature, combustion temperature, combustion rates, and ignition/combustion morphology can be determined. NASA will use the results to design safer components for launch vehicles, such as the Space Shuttle, which uses large quantities of liquid oxygen at high pressures. The results are also directly applicable to industrial handling of high pressure oxygen.

Thermal Properties of Advanced High-Temperature Materials

L.L. Sparks

Ceramics and ceramic based composites are becoming increasingly important as replacements for metals and plastics in electronic components and high performance engines and structures. The bulk of the developmental research on these materials has been in the areas of processing and mechanical properties.

Thermal properties must be known for advanced applications now being contemplated or, in some cases, actually incorporated in working designs.

The properties in question include thermal conductivity, thermal expansion, heat capacity, and thermal diffusivity. Knowledge of these properties is required to allow ceramics to be used in applications such as unlubricated bearings, high-temperature reactors, turbine rotors, adiabatic diesel engines, turbocompressors, thermal barriers, electrical components, and substrates for electronic components.

The initial effort at NBS to address the thermal properties needs is to develop a thermal conductivity apparatus with the capability to measure thermal conductivity of ceramic-like materials to 1000 °C. The apparatus will be a steady-state device, will accommodate specimens up to 6 cm in diameter and 1.3 cm thick, and will operate in either a gas or high vacuum environment. Design of the system has been completed and construction begun. Other agency funding is being sought to supplement in-house support in FY86. A cooperative program for utilization of this apparatus has been established with the Center for Ceramic Research at Rutgers University, and a tentative program established with the Advanced Materials Institute (Colorado School of Mines and several industrial subscribers).

A second apparatus is required to satisfy the very high temperature (1000 °C) thermal conductivity needs. Design of this system is now being considered; a transient technique will probably be chosen. Development of this system will follow proof testing of the steady-state system. Currently available apparatuses to study thermal expansion and heat capacity will be modified as required to allow use at high temperatures.

Oxidation of Metals in High Pressure/High Temperature Oxygen

J.W. Bransford, J.A. Hurley

A program to design and operate a Thermogravimetric apparatus (TGA) has been undertaken. The TGA apparatus, now in the design stage, will be used to directly determine the oxidation rate of various metal alloys in high-temperature/high-pressure oxygen.

The data generated by these studies will be of interest to all users of oxygen at high temperature and elevated pressure.

5. HONORS AND AWARDS

Howard J.M. Hanley - Department of Commerce, Gold Medal Award for his pioneering studies on fluids out of equilibrium, resulting in profound changes in understanding of nonlinear phenomena and new bases for design of chemical processes.

Richard D. Noble - The American Telephone and Telegraph Foundation Award of the American Society of Engineering Education for excellence in teaching engineering courses as an associate professor adjunct at the University of Colorado in Boulder.

Neil A. Olien - The Centennial 100 Alumni Award for outstanding accomplishments from the South Dakota School of Mines and Technology, March 1985.

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Rainwater, J.C. and Williamson, F.R., Vapor-liquid equilibrium of near-critical binary alkane mixtures, to be published in Int. J. of Thermophysics.

Rainwater, J.C., Hanley, H.J.M., Paskiewicz, T. and Petru, Z., Non-Newtonian flow of a model liquid between concentric cylinders, J. Chem. Phys., Vol. 83, No. 1, pp. 339-347 (July 1985).

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Sparks, L.L. and Arvidson, J.M., Thermal and mechanical properties of polyurethane foams at low temperatures, J. Ther. Insulation, Vol. 8, pp. 198-232 (Jan. 1985).

Steward, W.G., A centrifugal pump for superfluid helium, to be published in Cryogenics.

Straty, G.C. and Palavra, A.M.F., Automated high temperature PVT apparatus with data for propane, Nat. Bur. Stand. (U.S.) J. Res., Vol. 89, No. 5, pp. 375-383 (Sept.- Oct. 1984).

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Voth, R.O., Producing liquid-solid mixtures (slushes) of oxygen and hydrogen using an auger, to be published in Cryogenics.

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Younglove, B.A. and Hanley, H.J.M., The viscosity and thermal conductivity coefficients of gaseous and liquid argon, to be published in J. Phys. & Chem. Ref. Data.

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7. TALKS

Radebaugh, R., Regenerators for Magnetic Refrigeration, Workshop on Magnetic Refrigeration, Los Alamos, NM, Sept. 20, 1984.

Bruno, T.J., Instrumental Aspects of Supercritical Fluid Chromatography, Georgetown University, Washington, DC, Oct. 19, 1984.

Sparks, L.L., Thermal and Mechanical Properties of Polyurethane Foams at Cryogenic Temperatures, 28th Annual Polyurethane Division Technical/Marketing Conference, Society of the Plastics Industry, San Antonio, TX, Nov. 7, 1984.

Fox, J.R., Nonclassical Equations of State, Rice University, Houston, TX, Nov. 8, 1984.

Bruno, T.J., Direct Fugacity Measurements on Hydrogen Mixtures, Colorado School of Mines, Golden, CO, Nov. 9, 1984.

Siegwarth, J.D., Vortex Shedding Flowmeters for Space Shuttle Use, Chemical Engineering Science Division Colloquium, Boulder, CO, Nov. 9, 1984.

Bruno, T.J., Direct Fugacity Measurements on Hydrogen Mixtures, AIChE 1984 Annual Meeting, San Francisco, CA, Nov. 11, 1984.

Noble, R.D., Facilitated Transport of Gases Through Liquid Membranes, Rutgers University, Piscataway, NJ, Nov. 15, 1984.

Rainwater, J.C., Density Corrections to Gas Transport Properties: A Tentative Answer to a 67-year-old Problem, Chemical Engineering Science Division Colloquium, Boulder, CO, Nov. 20, 1984.

Larson, K.M., Carrier Enhanced Acetic Acid Extraction with Emulsion Liquid Membranes, AIChE 1984 Annual Meeting, San Francisco, CA, Nov. 26, 1984.

Noble, R.D., Mathematical Modeling of Facilitated Transport Membranes, Dow Chemical Co., Walnut Creek, CA, Nov. 27, 1984.

Ely, J.F., Statistical Mechanical Theory of Local Composition, AIChE 1984 Annual Meeting, San Francisco, CA, Nov. 28, 1984.

McManus, S.E., The Decay of Swirl in Turbulent Compressible Flow in a Long Pipe, Chemical Engineering Science Division Colloquium, Boulder, CO, Dec. 3, 1984.

Rainwater, J.C., Density Corrections to Transport Properties for Gases with Realistic Potentials, University of Florida, Gainesville, FL, Dec. 11, 1984.

McManus, S.E., The Decay of Turbulent Swirling Flows in a Long Pipe, American Gas Association Transmission Measurement Committee Meeting, Arlington, VA, Jan. 28, 1985.

Friend, D.G., Transport Properties in Fluids, University of Colorado, Denver, CO, Feb. 22, 1985.

Noble, R.D., Chemical Complexation Using Liquid Membranes, Chemical Engineering Science Division Colloquium, Boulder, CO, Mar. 22, 1985.

Noble, R.D. (Coauthors: Way, J.D. and Powers, L.A.), Boundary Layer Effects in Facilitated Transport of Liquid Membranes, AIChE Spring National Meeting, Houston, TX, Mar. 25, 1985.

Olien, N.A., Future Needs in Thermophysical Property Research: Experiment, Theory and Data Evaluation, AIChE Spring National Meeting, Houston, TX, Mar. 25, 1985.

Hanna, G.J. (Coauthor: Noble, R.D.), Measurement of Liquid-Liquid Interfacial Kinetics, AIChE Spring National Meeting, Houston, TX, Mar. 26, 1985.

Way, J.D. (Coauthors: Noble, R.D. and Reed, D.L.), Facilitated Transport of Carbon Dioxide in Ion-Exchange Membranes, AIChE Spring National Meeting, Houston, TX, Mar. 27, 1985.

Siegwarth, J.D., High Flow Velocity Vortex Shedding Flowmeter Design, NBS Vortex Shedding Consortium Meeting, NBS, Gaithersburg, MD, Mar. 28, 1985.

Noble, R.D., Modeling of Chemical Complexation in Liquid Membranes, Louisiana Tech. University, Ruston, LA, Mar. 29, 1985.

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Callanan, J.E., Internal Friction and Dynamic Young's Modulus of a Bituminous Coal, American Chemical Society, Miami, FL, Apr. 30, 1985.

McManus, S.E., The Decay of Swirling Gas Flow in Long Pipes, American Gas Association Distribution/Transmission Conference, Boston, MA, May 22, 1985.

Steward, W.G., The Use of a Remote Fusion Reactor as a Domestic Energy Source, Chemical Engineering Science Division Colloquium, Boulder, CO, May 31, 1985.

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Diller, D.E., Shear Viscosity Coefficients of Compressed Gaseous and Liquid Carbon Dioxide, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Sullivan, S.A., Experimental Determinations of Thermal Properties of Coal in Varying Atmospheres: Specific Heats and Heats of Desorption of Water, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Rainwater, J.C., Non-Newtonian Flow Between Concentric Cylinders and the Effects of Finite Compressibility, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Magee, J.W., Specific Heats [Cv] of Saturated and Compressed Liquid and Vapor Carbon Dioxide, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

McCarty, R.D., Extended Corresponding States, Is It a Viable tool for the Prediction of the Thermodynamic Properties of Mixtures, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Friend, D.G. (Coauthor: Roder, H.M.), The Thermal Conductivity of Methane-Ethane Mixtures at Temperatures between 140 and 330 K and at Pressures up to 70 MPa, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Olien, N.A., Evaluated Engineering Data from the National Bureau of Standards, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 26, 1985.

Rainwater, J.C., Vapor-Liquid Equilibrium of Near-Critical Binary Mixtures, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 26, 1985.

Roder, H.M. (Coauthor: Friend, D.G.), The Thermal Conductivity Enhancement in Three Binary Methane-Ethane Mixtures, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 26, 1985.

Bruno, T.J., Direct Fugacity Measurements on H_2/C_1, H_2/C_3, H_2/CO_2, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 26, 1985.

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Siegwarth, J.D., High Flow Velocity Vortex Shedding Flowmeter Design, NASA-MSFC, Huntsville, AL, June 27, 1985.

Noble, R.D., Gas Separations Using Chemical Complexation, du Pont Polymer Products Department, Experimental Station, Wilmington, DE, July 18, 1985.

Way, J.D., Facilitated Transport in Ion Exchange Membranes, du Pont Experimental Station, Polymer Products Department, Wilmington, DE, July 18, 1985.

Giarratano, P.J., Experiments in Zero-G on Board a NASA KC135, Boulder Kiwanis Club, Boulder, CO, July 18, 1985.

Louie, B., A Thermometer for Fast Response in Cryogenic Flow, 1985 Cryogenic Engineering Conference, Massachusetts Institute of Technology, Cambridge, MA, Aug. 13, 1985.

Haynes, W.M., Orthobaric Liquid Densities and Dielectric Constants of Carbon Dioxide, Cryogenic Engineering Conference, Massachusetts Institute of Technology, Cambridge, MA, Aug. 15, 1985.

Steward, W.G., A Centrifugal Pump for Superfluid Helium, NASA Helium Transfer in Space Workshop, NBS, Boulder, CO, Aug. 21, 1985.

Friend, D.G. (Coauthor: Roder, H.M.), Enhancement of the Thermal Conductivity Near the Liquid-Vapor Critical Line of Binary Methane-Ethane Mixtures, Gordon Research Conference on Physics and Chemistry of Liquids, Plymouth, NH, Aug. 21, 1985.

Friend, D.G. (Coauthor: Rainwater, J.C.), Theory of Viscosity and Thermal Conductivity of Dense Gases, Gordon Research Conference on Physics and Chemistry of Liquids, Plymouth, NH, Aug. 22, 1985.

Sullivan, S.A., Heat Capacity of Titanium from 320-560 K, Fortieth Calorimetry Conference, Pacific Grove, CA, Aug. 26, 1985.

Magee, J.W., Specific Heat [Cv] Measurements of Compressed Vapor and Liquid (Methane + Ethane) Mixtures, Fortieth Calorimetry Conference, Pacific Grove, CA, Aug. 26, 1985.

Bunge, A.L. (Coauthor: Noble, R.D.), Influence of Reversible Consumption on Continuous Flow Extraction by Emulsion Liquid Membranes, AIChE Summer National Meeting, Seattle, WA, Aug. 26, 1985.

Baird, R.S. (Coauthors: Bunge, A.L. and Noble, R.D.), Batch Extraction of Amines Using Emulsion Liquid Membranes--Importance of Reaction Reversibility, AIChE Summer National Meeting, Seattle, WA, Aug. 27, 1985.

Callanan, J.E., The Gamma-Gamma and Melting Transitions in a Hafnium-Bearing Superalloy, Fortieth Calorimetry Conference, Pacific Grove, CA, Aug. 27, 1985.

Filla, B.J., Heats of Desorption from Porous Solids, Fortieth Calorimetry Conference, Pacific Grove, CA, Aug. 28, 1985.

Callanan, J.E., Reversible Effects in Heat Capacity Measurements of Insulations, Fortieth Calorimetry Conference, Pacific Grove, CA, Aug. 29, 1985.

Hiza, M.J., Data for the Chemical Industry: An Overview of International Data Projects and Quality Control of Computerized Thermophysical Property Data Bases, International Meetings on Phase Equilibria and Related Property Data, Universitaire de Paris, Paris, France, Sep. 9, 1985.

Baltatu, M.--Fluor Corp. (Coauthors: Olien, N.A. and Hanley, H.J.M.), Thermophysical Properties Data Bases: A Realistic Assessment from the Industrial-Academic Viewpoint, International Meetings on Phase Equilibria and Related Property Data, Universitaire de Paris, Paris, France, Sep. 9, 1985.

Noble, R.D., Model of a Cellular Bioreactor for Cellobiosic Hydrolysis, ENEA, Laboratorio Chimica Applicata, Rome, Italy, Sep. 17, 1985.

Noble, R.D., Modeling of a Biomedical Reactor for Pancreas: Stability, Duration, and Biocompatibility, ENEA, Laboratorio Chimica Applicata, Rome, Italy, Sep. 19, 1985.

McManus, S.E., The Decay of Swirl, Colorado School of Mines, Golden, CO, Oct. 3, 1985.

Perkins, R.A., Calorimetry of Natural Gas Hydrates, Colorado School of Mines, Golden, CO, Oct. 9, 1985.

Way, J.D. (Coauthors: Noble, R.D. and Powers, L.A.), Facilitated Transport of Acid Gases in Ion Exchange Membranes, ACS Pacific Conference on Chemistry and Spectroscopy, San Francisco, CA, Oct. 10, 1985.

Callanan, J.E., Effects of Desorption of Water During Heat Capacity Measurements of Raw Coals, Electrochemical Society Meeting, Las Vegas, NV, Oct. 15, 1985.

Noble, R.D., An Overview of Membrane Separations, Fourth Symposium on Separation Science and Technology for Energy Applications, Knoxville, TN, Oct. 24, 1985.

Fox, J.R., Forth What Is?, Chemical Engineering Science Division Colloquium, Boulder, CO, Oct. 25, 1985.

Siegwarth, J.D., High Flow Velocity Vortex Shedding Flowmeter Design, The NBS Vortex Shedding Consortium Meeting, NBS, Gaithersburg, MD, Oct. 31, 1985.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

J.A. Brennan

Amer. Gas Assoc. Transmission Measurement Committee (Technical Advisor)

OIML, U.S. National Working Group, SP5P/SR2 (Member)

D.E. Daney

Boulder Editorial Review Board (Member)

R.D. Noble

American Society for Engineering Education (ASEE), Chemical Engineering Division (Member)

Gordon Conference on Separation and Purification (Vice Chairman 1986, Chairman 1987)

ASEE Rocky Mountain Section 1984 (Program Chairman)

R.O. Voth

Division 773 Hazards Review Committee (Chairman)

M.J. Hiza

AIChE National Cryogenics Committee, 13h

CODATA Task Group on Data for the Chemical Industry (Member)

J. Hord

AIChE Research Committee (Member and Chairman of Oversight Subcommittee)

AIChE Government Programs Steering Committee (Liaison to Research Committee)

D.E. Diller

ASTM D-3 Gaseous Fuels Committee, Thermophysical Properties Subcommittee (Member)

J.F. Ely

AIChE Program Committee Area 1-a, Thermodynamics and Transport Properties (Chairman)

Gas Processors Association Data Book Revision Committee (Member)

AIChE/DIPPR Technical Committee 802 (Member)

NBS/NEL Technical Evaluation Committee (Member)

D.G. Friend

Boulder Editorial Review Board (Member)

H.J.M. Hanley

ASME Thermophysical Properties Committee (Chairman)

International Union of Pure and Applied Chemistry Committee on Quantum Fluids (Member)

International Union of Pure and Applied Chemistry Commission on Transport Properties (Member)

R.D. McCarty

AIChE/DIPPR Vapor Pressure and Density Subcommittee (Member)

N.A. Olien

ASTM D-3 Gaseous Fuels (Member)

Gas Research Institute Steering Committee on Revision of AGA 3/NX-19 (Member)

IUPAC Committee on Transport Properties (Corresponding Member)

Program Committee, International Symposium on Fluid Flow Measurements (Member)

H.M. Roder

International Union of Pure and Applied Chemistry Committee on Quantum Fluids (Member)

NBS Computer Advisory Committee (Member)

NBS-NOAA - Joint Computer Advisory Committee (Member)

B.A. Younglove

Division 773 Hazards Review Committee (Member)

J.W. Bransford

ASTM G4 Committee on Materials Compatibility and Sensitivity in Oxygen Enriched Atmosphere, Test Methods Subcommittee (Member)

Division 773 Hazards Review Committee (Member)

J.E. Callanan

Calorimetry Conference Board of Directors (Director)

Calorimetry Conference Standards Committee (Member)

ASTM E37 on Thermal Measurements, Test Methods and Recommended Practices Subcommittee (Member), and Standard Reference Materials Subcommittee (Chairman)

American Chemical Society, Fuel Division (Membership Chairman)

ACS Regional Meeting, Symposium Co-chairman, 1986

J.G. Hust

ASTM C16 on Thermal Insulations, Thermal Measurements Subcommittee (Member)

ASTM E37 on Thermal Measurements, Standard Reference Materials Subcommittee (Member)

International Thermal Conductivity Conference (Member of Governing Board)

R. Radebaugh

Federal Government Interagency Panel on Refrigeration (Member)

Cryogenic Engineering Conference Board (Chairman)

Conference on Cryocoolers--1986 (Program Committee)

L.L. Sparks

ASTM E20 on Temperature Measurement, Thermocouples Subcommittee (Member)

ASTM C16 on Thermal Insulation, Thermal Measurement Subcommittee (Member)

ASTM C9 on Concrete and Concrete Aggregates (Member)

S. A. Sullivan

Rocky Mountain Thermal Analysis Forum, Board of Directors (Chairman)

EDITORSHIPS

J.D. Way

Journal of Membrane Science, Proceedings of the Membrane Separation Technology Symposia at the 1983 Denver AIChE Meeting (Guest Editor), Vol. 21, pp. 1-112 (1984)

H.J.M. Hanley

NBS Journal of Research (Boulder Editor)

International Journal of Thermophysics (Editorial Board)

W.M. Haynes

Cryogenics (U.S. Advisory Editor)

M.J. Hiza

Fluid Phase Equilibria (Editorial Board)

N.A. Olien

Journal of Physical and Chemical Reference Data (Editorial Board)

J.G. Hust

Review of Scientific Instruments (Editorial Board)

Journal of Thermal Insulation (Editorial Board)

9. PROFESSIONAL INTERACTIONS

FACULTY APPOINTMENTS

M.C. Jones
Adjunct Associate Professor, Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines

R.D. Noble
Associate Professor Adjunct, Department of Chemical Engineering, University of Colorado

J.F. Ely
Adjunct Professor, Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines

H.J.M. Hanley
Professor Adjoint, Department of Chemical Engineering, University of Colorado

M.J. Hiza
Adjunct Professor, Department of Chemical Engineering, University of Wyoming

J.C. Rainwater
Associate Professor Adjoint, Department of Physics, University of Colorado

INDUSTRY

B.R. Bateman
Cooperative Research with M.D. Freeman, the Foxboro Company, Foxboro, MA, on flow measurement.

Consultation with F.W. Sullivan, Chairman, Gas Research Institute Basic Gas Metering Committee, Brooklyn Union Gas Co., Brooklyn, NY, on natural gas custody transfer.

Consultation with S. Walker, Goodflow Products, Tulsa, OK, on the design of experimental orifice meters.

Consultation with H.W. Fisher, Manager, Gas Products Engineering/Research, Rockwell International, Pittsburgh, PA, on the design of experimental orifice meters.

Consultation with D.D. Barnes, Fluidic Techniques, Mansfield, TX, on the design of experimental meters.

J.A. Brennan
Consultation with N.A. Verini, Airco Industrial Gases, Murray Hill, NJ, on CGA flow measurement standards.

Consultation with F.W. Sullivan, Chairman, Gas Research Institute Basic Gas Metering Committee, Brooklyn Union Gas Company, Brooklyn, NY, on custody transfer of natural gas.

Consultation with C. Griffis and R. Norman, Gas Research Institute, Chicago, IL, on flow measurement research.

D.E. Daney
Consultation with J. Dillard, Barber-Nichols Engineering Company, Denver, CO, on cryogenic pumps.

Consultation with B.W. Birmingham, B.W. Birmingham Associates, Boulder, CO, on cryogenic heat transfer.

D.M. Ginley
Consultation with D. Dickey, Chemineer Co., Dayton, OH, on the design and selection of mixing equipment and key measurements for a 100 to 300 gallon capacity experimental facility.

Consultation with J. Oldshue, Mixco, Rochester, NY, on the design and selection of mixing equipment and key measurements for a 100 to 300 gallon capacity experimental facility.

K.M. Larson
Consultation with P. Mattison, Henkel Corporation, Minneapolis, MN, on complexing agents in separation processes.

Consultation with R. Busche, du Pont Co., Wilmington, DE, on acetic acid recovery.

Consultation with R. Eltz, Monsanto Co., St. Louis, MO, on separations of proteins.

D.B. Mann
Consultation with F.W. Sullivan, Chairman, Gas Research Institute Basic Gas Metering Committee, Brooklyn Union Gas, Brooklyn, NY, on custody transfer of natural gas.

Consultation with L. Bell, GIIGNL, Western LNG Corp., Los Angeles, CA, on metrology of liquefied natural gas.

Consultation with P. Hoglund, Chairman, AGA Gas Custody Transfer Committee, Washington Natural Gas, Seattle, WA, on orifice metering of natural gas.

Cooperative research with R. Norman, Gas Research Institute, Chicago, IL, on flow metering research.

S.E. McManus
Collaborative research with C. Griffis, Gas Research Institute, Chicago, IL, on the decay of turbulent, compressible swirling flow in long pipes.

D.L. Reed
Consultation with J. Mosely, Dow Chemical Co., Walnut Creek, CA, on polymeric and ion exchange membrane applications in the gas industry.

S.K. Sikdar
Consultation with D. Woodruff, General Electric Company, Schenectady, NY, on chemical vapor deposition.

Consultation with M. Mickley, Independent Consultant, Boulder, CO, on the water shortage problem and membrane transport.

Consultation with A. Michaels, President, Alan D. Michaels, Inc., Boston, MA, on biochemical separation.

C.F. Sindt

Consultation with W. Siedl and C. Briton, Colorado Engineering Experimental Station, Nunn, CO, on flow measurement.

Consultation with J. Jones and G. Less, Natural Gas Pipeline Company of America, Joliet, IL, on natural gas flow measurement.

Consultation with personnel of Colorado Interstate Gas, Denver, CO, on natural gas flow measurement.

W.G. Steward

Consultation with Creare, Inc., Hanover, NH, on helium cooled coils.

I. Vazquez

Consultation with E.E. Buxton, Flow Measurement Consultant, St. Albans, WV, on Ohio State University water tests data base.

Consultation with W.A. Fling, Vice-President, Cities Services R & D Corporation, Tulsa, OK, on Ohio State University water tests data base.

J.D. Way

Cooperative research with U. Bonne and D. Deetz of the Honeywell Physical Sciences Center, Minneapolis, MN, on chemically based sensors.

Consultation with D. Roberts, SRI International, Menlo Park, CA, on membrane technology.

J.F. Ely

Cooperative research with M.E. Baltatu, Fluor Engineering Inc., Irvine, CA, on properties of petroleum fractions and coal liquids.

Technical Manager of industrial consortium, consultation with member companies involved: Air Products and Chemicals, Inc., Allied Chemical Corporation, Amoco Production Company, ARCO Transportation Company, Cooper Energy Services, E.I. du Pont de Nemours and Company, Gas Processors Association, Mobil Research and Development Corporation, Monsanto Company, Phillips Petroleum Company, Shell Development Company, SOHIO, Texaco Inc., and Ingersoll-Rand Company, on prediction of fluid properties.

Cooperation with staff of the Gas Processors Association, Tulsa, OK, and the Gas Research Institute, Chicago, IL, on fluid properties predictions.

H.J.M. Hanley

Cooperative research with J.A. Barker, IBM, San Jose, CA, on theory of fluids and molecular dynamics.

Cooperative research with M.E. Baltatu, Fluor Engineering, Inc., Irvine, CA, on properties of petroleum fractions and coal liquids.

Cooperation with staff of the Gas Research Institute, Chicago, IL, on fluid properties predictions.

M.J. Hiza

Consultation with D.B. Crawford, M. W. Kellogg, Houston, TX, AIChE Committee 13h, on unit operations topics.

Consultation with T. Selover, SOHIO R&D, Cleveland, OH, on data for the petrochemical industry and his participation in the activities of the CODATA Task Group on Data for the Chemical Industry.

Consultation with S.C. Paspek, SOHIO R&D, Cleveland, OH, on industrial interest in heat transfer, experiments and models, to solute laden supercritical solvents.

Consultation with L. Sobel, Atochem, Paris, France, on CODATA activities--data compilations for the chemical industry.

Consultation with C.F. Spencer, M.W. Kellogg, Houston, TX, on CODATA activities--data compilations for the chemical industry.

Consultation with D. Zudkevitch, Allied Chemical Corp., Morristown, NJ, on appropriate CODATA guidelines for the reporting of phase equilibria data for industrial chemicals data bases.

Consultation with M.E. Baltatu, Fluor Engineering Inc., Irvine, CA, on her participation in the activities of the CODATA Task Group on Data for the Chemical Industry.

Consultation with W.J. Ward, General Electric Co., Schenectady, NY, on current directions and interests in separations research.

J.W. Magee

Consultation with steering committee of industrial consortium whose member companies are: Air Products and Chemicals, Inc., Allied Chemical Corporation, Amoco Production Company, ARCO Transportation Company, Cooper Energy Services, E.I. du Pont de Nemours and Company, Gas Processors Association, Mobil Research and Development Corporation, Monsanto Company, Phillips Petroleum Company, Shell Development Company, SOHIO, Texaco Inc., Ingersoll-Rand Company, on measurements of fluid properties.

N.A. Olien

Consultation with L.J. Kemp, So. California Natural Gas, Los Angeles, CA, on standardization of thermophysical properties of natural gas constituents.

Consultation with R. Tefankjian, Texas Eastern Transmission Co., Houston, TX, on property data for natural gas measurement.

Consultation with S.C. Paspek, SOHIO, Cleveland, OH, on properties of supercritical solvents.

Consultation with W. Barlen, Compressed Gas Association, Arlington, VA, on custody transfer of industrial gases.

Consultation with M. Klein, Gas Research Institute, Chicago, IL, on properties of fluids.

J.C. Rainwater

Collaborative research with P.M. Holland, Proctor & Gamble, Cincinnati, OH, on transport properties of fluids.

B.A. Younglove

Consultation with W.R. Dagle, Applied Technologies Inc., Boulder, CO, on sound speeds and measurement techniques.

Consultation with P. Banks, Big Three Industries, Houston, TX, on thermodynamic properties calculations.

Consultation with M. Thompson, Interstate Technologies, Walwick, NJ, on sound speed measurements in water.

Consultation with T.D. Russos, Industrial Materials Technology, Andover, MA, on argon gas pressurization in metallic powder processing.

Consultation with D. Smith, Liquid Air Corporation, San Francisco, CA, on thermodynamic properties and computer programs.

Consultation with J. Schrecongask, ANSUTECH, King of Prussia, PA, on thermophysical properties.

Consultation with B. Titman, Rockwell International Science Center, Thousand Oaks, CA, on sound speed measurement techniques in nitrogen, oxygen, and their mixtures.

J.E. Callanan

Consultation with S.C. Mraw, Exxon Corporate Research, Houston, TX, on thermal measurements on coal.

Consultation with C.T. Ratcliffe, Union Oil Research, Brea, CA, on thermal measurements on coal.

Consultation with E. Spearin, Inland Steel, East Chicago, IN, on thermal property measurements of coal.

J.G. Hust

Consultation with C.M. Pelanne, CMP Consultant, Denver, CO, on thermal insulation standards.

Consultation with H. Mitchell, Manville Corp., Denver, CO, on thermal insulation standards.

Consultation with R.P. Tye, Dynatech R&D Co., Cambridge, MA, on low conductivity thermal Standard Reference Materials.

R. Radebaugh

Consultation with S. Russo, Hughes Aircraft, El Segundo, CA, on regenerator efficiency studies.

L.L. Sparks

Consultation with R.P. Tye, Dynatech R&D Co., Cambridge, MA, on ASTM standards.

Consultation with R.W. Rosser, Hughes Aircraft, Culver City, CA, on friction and wear of composites.

Consultation with J. Segal, Zeiss Inc., Thornwood, NY, on optical characterization of solids.

S.A. Sullivan

Cooperative research with P. Dempsey, CAD/CAM Applications, Boulder, CO, on thermal properties of terpolymers.

ACADEME, NATIONAL LABORATORIES AND GOVERNMENT

V.D. Arp

Collaborative research with R.B. Owen, NASA-MSFC, Huntsville, AL, on optical measurements and zero-g heat transfer measurements.

Consultation with T. Cleghorn, NASA-JSC, Houston, TX, on hydrogen-oxygen mixing.

Consultation with B. Hands, Oxford University, Oxford, England, on useful forms of fluid state equations.

Consultation with P. Kittel, NASA-ARC, Moffet Field, CA, on helium pumps for space flight.

S.D. Bischke

Consultation with P. Glugla, Dept. of Chemical Engineering, University of Colorado, Boulder, CO, on amino acid transport through ionomeric membranes.

J.A. Brennan

Consultation with E. Jenkins, California State Dept. of Agriculture, Division of Measurement Standards, Sacramento, CA, on flow measurement standards.

Consultation with F. Kinghorn, National Engineering Laboratory, East Kilbride, Scotland, on flow measurement.

D.E. Daney

Cooperative research with L.P. Purtell, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on modeling of fluid tangential vortex motion in cylindrical tanks near zero-g for mechanically induced fluid transfer between tanks.

P.J. Giarratano

Collaborative research with R.B. Owen, NASA-MSFC, Huntsville, AL, on transient heat transfer experiments near zero-g.

Collaborative research with A. Cezairliyan and A. Miiller, Thermophysics Division , NBS/CCE, Gaithersburg, MD, on thermophysical measurements in reduced gravity.

D.M. Ginley

Collaborative research with S.J. Khang, Dept. of Chemical Engineering, University of Cincinnati, Cincinnati, OH, on bench-scale mixing tests.

Collaborative research with D. Friday, Statistical Engineering Division, NBS/CAM, Boulder, CO, on analysis of mixing data.

G.J. Hanna

Cooperative research with A.L. Bunge, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on distribution coefficient enhancement in thin oil films in emulsions and on amine neutralization using emulsion liquid membranes.

Consultation with R.H. Guy, School of Pharmacy, University of California, San Francisco, CA, on the rotating diffusion cell and interfacial kinetics measurement.

Consultation with P.R. Danesi, Argonne National Laboratory, Argonne, IL, on interfacial kinetics measurement.

Consultation with M. Kreevoy, Dept. of Chemistry, University of Minnesota, Minneapolis-St. Paul, MN, on interfacial kinetics models and measurements.

Consultation with R. Bartsch, Dept. of Chemistry, University of Texas, Austin, TX, on interfacial kinetics measurements in ionizable crown ether systems.

Consultation with J. Lamb, Dept. of Chemical Engineering, Brigham Young University, Provo, UT, on interfacial kinetics in crown ether systems.

K.M. Larson

Cooperative research with A.L. Bunge, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on amine neutralization and copper extraction using emulsion liquid membranes.

Consultation with J. Draxler, Technical University of Graz, Graz, Austria, on particle-size measurement of emulsion liquid membranes.

Consultation with T.A. Hatton, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, on separation of proteins.

Consultation with A. Carlson, Dept. of Chemical Engineering, Penn State University, University Park, PA, on aqueous two-phase extraction of proteins.

B. Louie

Cooperative research with T. Cleghorn, NASA-JSC, Houston, TX, on cryogen storage and transfer.

Collaborative research with T. Lenz, Dept. of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO, on cryogenic propellant scavenging.

D.B. Mann

Consultation with F.C. Kinghorn and W.C. Pursley, National Engineering Laboratory, East Kilbride, Scotland, on orifice meter research.

R.D. Noble

Cooperative research with A.L. Bunge, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on mathematical modeling and experiments for emulsion liquid membrane separations.

Cooperative research with C.A. Koval, Dept. of Chemistry, University of Colorado, Boulder, CO, on experiments related to facilitated transport of gases across liquid films.

Cooperative research with T.A. Hatton, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, on modeling of separations in chemically reactive systems.

Cooperative research with P. Danesi, Argonne National Laboratory, Argonne, IL, on modeling of facilitated transport in hollow fiber membranes.

Consultation with ENEA Laboratories, Rome, Italy, on setting up a collaborative research program in gas separations and enzyme reactors.

R.A. Perkins

Cooperative research with A.J. Kidnay, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on titration and flow calorimetry.

Cooperative research with B.E. Dale, Dept. of Agricultural and Chemical Engineering, Colorado State University, Ft. Collins, CO, on thermodynamics of protein denaturation.

Cooperative research with S. Selim, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on diffusion of macromolecules.

L.A. Powers

Collaborative research with D. Nilsen, U.S. Bureau of Mines, Albany Research Center, Albany, OR, on solvent extraction modeling.

Collaborative research with M. Bier, Center for Separation Science, Univ. of Arizona, Tucson, AZ, on supercritical chromatography in space.

D.L. Reed

Cooperative research with A.L. Bunge, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on mathematical modeling and experiments in emulsion liquid membranes.

Cooperative research with C.A. Koval, Department of Chemistry, University of Colorado, Boulder, CO, on experiments related to facilitated transport of gases through liquid films.

Consultation with Jin, M.F., Dalian Institute of Chemical Physics, Dalian, China, on organic acid and metal extraction using emulsion liquid membranes.

S.K. Sikdar

Collaborative research with M. Bier, Center for Separation Science, University of Arizona, Tucson, AZ, on separation of organic and biomaterials in space.

Collaborative research with A.D. Randolph, Dept. of Chemical Engineering, University of Arizona, Tucson, AZ, on crystallization of organic and biochemicals in space.

Collaborative research with B. Dale, Dept. of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO, on denaturation of proteins.

Collaborative research with S. Selim, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on the measurement of diffusivities of proteins and chemicals.

Collaborative research with P. Glugla, Dept. of Chemical Engineering, University of Colorado, Boulder, CO, on the transport of organic species through ion-exchange membranes.

Consultation with C. McConica, Dept. of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO, on chemical vapor deposition.

Collaborative research with H. Semerjian, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on the measurement of amino acids using two-dimensional spectroscopy.

Consultation with T.K. Ghose, Distinguished Visiting Professor, University of Delaware, Newark, DE, on biochemical engineering problems.

Consultation with D. Kampala, Dept. of Chemical Engineering, University of Colorado, Boulder, CO, on fermentation reactor modeling.

W.G. Steward

Consultation with A. Rodriquez at Kennedy-KSC, J.F. Kennedy Space Center,FL, on orifice flowmeter operation for hydrogen flare system.

Consultation with Y.S. Ng at NASA-ARC, Moffet Field, CA, on cryogenic system cooldown and centrifugal pump characteristics.

Consultation with F. Edeskuty, Los Alamos National Laboratory, Los Alamos, NM, on cryogenic system flow stability and cooldown.

C.F. Sindt

Cooperative research with J.R. Whetstone, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on the acquisition and analysis of orifice meter data for natural gas in the Natural Gas Pipeline of America Company facility in Joliet, IL.

R.O. Voth

Consultation with R.S. Carter, NBS/CRR, Gaithersburg, MD, on helium refrigerator capacity for the cold neutron program.

J.D. Way

Cooperative research with C.A. Koval, Dept. of Chemistry, University of Colorado, Boulder, CO, on facilitated transport of carbon monoxide.

Cooperative research with D. Nelson, Pacific Northwest Laboratories, Richland, WA, on complexation-based separation processes.

Cooperative research with C. Fabiani, ENEA Laboratories, Rome, Italy, on membrane technology.

Cooperative research with P. Glugla, Dept. of Chemical Engineering, University of Colorado, Boulder, CO, on facilitated transport using ion exchange membranes.

M.J. Hiza

Consultation with E.D. Sloan, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on importance of interpersonal relations and communication in an R&D organization.

Consultation with T.H.K. Frederking, Dept. of Chemical, Nuclear and Thermal Engineering, University of California, Los Angeles, CA, on AIChE Committee 13h work.

Consultation with A.M. Szafranski, Instytut Chemii Przemyslowei, Warsaw, Poland, on CODATA Task Group activities--data compilations for the chemical industry.

Consultation with A.S. Myers, Dept. of Chemical Engineering, University of Pennsylvania, Philadelphia, PA, on adsorption research.

Consultation with F. Howard, NASA-KSC, J.F. Kennedy Space Center, FL, on refrigeration/liquefaction, and phase equilibria thermodynamics.

Consultation with R.W. Fast, Fermilab, Batavia, IL, on Cryogenic Engineering Conference programs and a variety of CEC Board matters.

Consultation with B. LeNeindre, Laboratoire des Interactions Moleculaires et des Hautes Pressions, Universite Paris Nord-CNRS, Villetaneuse, France, on CODATA Task Group activities related to data projects important to the chemical industry.

Consultation with R.P. Danner, Dept. of Chemical Engineering, Pennsylvania State University, University Park, PA, on CODATA Task Group activities for '85-'86 related to data base projects.

Consultation with J.R. Whetstone, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on calculation of natural gas properties required for gas mixture orifice metering.

Consultation with H.G. Semerjian, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on optical techniques for analysis of biomolecules in solution.

Consultation with G. Mattingly, Chemical Process Metrology Division, NBS/CCE, Gaithersburg, MD, on experimental measurement needs for fluid management in microgravity environments.

Consultation with H.V. Kehiaian, Institute de Topologie et de Dynamique des Systemes, Universite Paris VII-CNRS, Paris, France, on technical programs and session chairpersons for three consecutive international conferences on phase equilibria and related properties.

Consultation with C. Young, Dept. of Physical Chemistry, University of Melbourne, Parkville, Australia, on critical evaluation of phase equilibria data for the IUPAC Solubility Data Series.

Consultation with G. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Murdoch, Australia, on collaboration in critical evaluation of phase equilibria data for the IUPAC Solubility Data Series.

T.J. Bruno

Consultation with L. Dickens, Denver Regional Council of Governments, Denver, CO, on statistical analysis.

Consultation with D.E. Martire, Dept. of Chemistry, Georgetown University, Washington, DC, on supercritical fluid chromatography.

D.E. Diller

Cooperative research with L. Van Poolen, Engineering Department, Calvin College, Grand Rapids, MI, and F. Santos, Instituto Superior Tecnico, Lisbon, Portugal, on measurements of viscosity of compressed gaseous and liquid mixtures.

J.F. Ely

Cooperative research with T. Leland, Dept. of Chemical Engineering, Rice University, Houston, TX, on hard sphere expansion theory for polar and nonpolar fluid mixtures.

Cooperative research with A. Mansoori, Dept. of Chemical Engineering, University of Illinois, Chicago, IL, on local composition models for fluid thermodynamic behavior.

Cooperative research with K.R. Hall, Thermodynamics Research Center, Texas A&M, College Station, TX, on new correlation of saturation properties of pure fluids.

Consultation with E.D. Sloan, A.J. Kidnay, and V. Yesavage, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on thermal conductivity of coal liquids.

Consultation with D.J. Evans, Research School of Chemistry, Australian National University, Canberra, Australia, on computer simulation.

D.G. Friend

Consultation with H. Meyer, Dept. of Physics, Duke University, Durham, NC, on thermal conductivity enhancement in mixtures.

H.J.M. Hanley

Cooperative research with A.J. Kidnay, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on properties of coal liquids.

Consultation with K. Gubbins, School of Chemical Engineering, Cornell University, Ithaca, NY, on transport properties of fluids.

Consultation with J. Kestin, Dept. of Mechanical Engineering, Brown University, Providence, RI, on transport properties of fluids.

Cooperative research with S. Hess, Dept. of Physics, Technical University of Berlin, West Germany, on structure of liquids.

Cooperative research with D. Evans, Research School of Chemistry, Australian National University, Canberra, Australia, on non-Newtonian phenomena.

Consultation with W.A. Wakeham, Dept. of Chemical Engineering, Imperial College, London, England, on transport phenomena.

Cooperative research with N.A. Clark, Dept. of Physics, University of Colorado, Boulder, CO, on behavior of colloidal suspensions.

Cooperative research with R. Hayter, Oak Ridge National Laboratory, Oak Ridge, TN, on neutron scattering from liquids.

W.M. Haynes

Cooperative research with J.C. Holste, Dept. of Chemical Engineering, Texas A&M, College Station, TX, on thermophysical properties of fluids.

Collaborative research with R. Masui, National Research Laboratory of Metrology, Ibaraki, Japan, on fluid densimetry.

Consultation with D.W. Kupke, Dept. of Biochemistry, University of Virginia, Charlottesville, VA, on magnetic suspension densimetry and viscometry.

Cooperative research with L. Van Poolen, Engineering Department, Calvin College, Grand Rapids, MI, on coexistence densities and liquid volume fractions.

J. W. Magee

Cooperative research with R. Kobayashi, Dept. of Chemical Engineering, Rice University, Houston, TX, on measurements of fluid mixture properties.

Consultation with J. Stecki, Polish Academy of Sciences, Warsaw, Poland, on measurement of fluid heat capacities.

R.D. McCarty
Collaborative research with R.T. Jacobsen, Dept. of Mechanical Engineering, University of Idaho, Moscow, ID, and Max Klein, Gas Research Institute, Chicago, IL, on equation of state research.

Collaborative research with R.T. Jacobsen, Dept. of Mechanical Engineering, University of Idaho, Moscow, ID, on ethylene properties.

Consultation with staff at the NASA-KCS, J.F. Kennedy Space Center, FL, on thermophysical properties of fluids.

Consultation with staff at the NASA-JSC, Houston, TX, on cryogenic fluid handling on the shuttle.

N.A. Olien
Consultation with K.R. Hall, Thermodynamics Research Center, Texas A&M University, College Station, TX, on properties of fluids and orifice metering of natural gas.

Consultation with K.E. Starling, School of Chemical Engineering and Material Science, Oklahoma University, Norman, OK, on equation of state.

Consultation with R. Wellek, National Science Foundation, Washington, DC, on thermophysical Properties.

J.C. Rainwater
Collaborative research with S. Hess, Dept. of Physics, Technical University of Berlin, West Germany, on theory of non-Newtonian liquids.

Cooperative research with M.R. Moldover, and J.M.H. Levelt Sengers, Thermophysics Division, NBS/CCE, Gaithersburg, MD, on thermodynamics of near-critical binary mixtures.

Cooperative research with L. Biolsi, Dept. of Chemistry, University of Missouri, Rolla, MO, on transport properties of fluids.

Cooperative research with L. Van Poolen, Engineering Dept., Calvin College, Grand Rapids, MI, on liquid volume fractions of mixtures.

Consultation with J. Dufty, Dept. of Physics, University of Florida, Gainesville, FL, on kinetic theory of liquids.

H.M. Roder

Consultation with W.A. Wakeham, Dept. of Chemical Engineering, Imperial College, London, England, on thermal conductivity of fluids.

Consultation with M.S. Graboski and E.D. Sloan, Dept. of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on thermal conductivity of fluids.

Cooperative research with C.A. Nieto de Castro, Dept. of Chemistry, University of Lisbon, Portugal, on measurements of thermal conductivity.

Cooperative research with J. Vernart, Dept. of Mechanical Engineering, University of New Brunswick, Canada, on thermal conductivity.

G.C. Straty

Cooperative research with A. Palavra, Interdisciplinary Institute, Technical University of Lisbon, Portugal, on measurements of fluids properties.

B.A. Younglove

Consultation with E. Jenkins, Department of Measurement Standards, Department of Agriculture, Sacramento, CA, on gas volumes for industrial standards.

J.W. Bransford

Consultation with D. Pippen, NASA-JSC, Houston, TX, and White Sands Test Facility, White Sands, NM, on oxygen safety procedures.

Consultation with C. Byrant, NASA-KSC, FL, on oxygen safety procedures.

J.E. Callanan

Consultation with J. Boerio-Goates, Dept. of Chemistry, Brigham Young University, Provo, UT, on calorimetric measurements.

Cooperative research with R.W. Carling, Sandia National Laboratory, Livermore, CA, on solid fuels thermal measurements.

Consultation with D. Merrick, Coal Research Establishment, UK, on thermal measurements of coal.

Consultation with A.J. Head, National Physical Laboratory, Teddington, UK, on DSC methods and standards.

Collaborative research with R. Weir, Royal Military College, Kingston, Ontario, Canada, on adiabatic calorimetry of solids.

Collaborative research with J. Crelling, Dept. of Geology, Southern Illinois University, Carbondale, IL, on solid fuels thermal measurements.

Collaborative research with R.A. McDonald and R.D. Mountain, Thermophysics Division, NBS/CCE, Gaithersburg, MD, on solid fuels properties modeling.

Consultation with S.B. Barton, Royal Military College, Kingston, Canada on measurements on coals.

Cooperative research with P. Roth, Sandia National Laboratory, Albuquerque, NM, on differential scanning calorimetry.

Collaborative research with E.F. Westrum, Jr., Dept. of Chemistry, University of Michigan, Ann Arbor, MI, on adiabatic calorimetry of solids.

J.G. Hust

Cooperative research with T. Ashworth and D. Smith, Dept. of Physics, South Dakota School of Mines and Technology, Rapid City, SD, on thermal insulations and geological materials research.

Consultation with F. Cabannes, CNRS, Orleans, France, on low conductivity Standard Reference Materials research.

Consultation with T. Faison and B. Rennex, NBS/CBT, Gaithersburg, MD, on thermal insulation standard reference materials.

R. Radebaugh

Consultation with G. Walker, Dept. of Mechanical Engineering, Calgary University, Calgary, Canada, on low temperature refrigeration.

Consultation with J. Barclay, Los Alamos National Laboratory, Los Alamos, NM, on regenerator efficiency studies and magnetic refrigeration.

L.L. Sparks

Consultation with R. Barkley, Dept. of Chemistry, University of Colorado, Boulder, CO, on thermal/mechanical properties of plastic foam insulations.

Consultation with J.B. Wachtman, Center for Ceramics Research, Rutgers University, Piscataway, NJ, on thermal properties of ceramics.

Consultation with M. Rhodes, Dept. of Chemistry, University of Massachusetts, Amherst, MA, on characterization of expanded plastics.

S.A. Sullivan

Cooperative research with N. Thedhani, Dept. of Mechanical Engineering, California Institute of Technology, Pasadena, CA, on thermal properties of alloys.

Collaborative research with F. Ramirez, Dept. of Chemical Engineering, University of Colorado, Boulder, CO, on heat capacity of lignite.

Collaborative research with J. Crelling, Dept. of Geology, Southern Illinois University, Carbondale, IL, on thermal property measurements of coal.

Collaborative research with D. Vecchia, NBS/CAM, Boulder, CO, on Standard Reference Materials development.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

A Symposium on Current Status and Future Trends in Thermophysical Property Research at the AIChE Spring National Meeting in Houston, TX, Mar. 24-28, 1985 was organized and chaired by N.A. Olien and M. Klein (GRI).

Cosponsored with ASME and the International Thermophysics Congress, the Ninth Symposium on Thermophysical Properties, held in Boulder, CO, Jun. 23-27, 1985. Organized and directed by H.J.M. Hanley.

Three International Meetings on Phase Equilibrium and Related Property Data, cosponsored by IUPAC, CODATA, and Universite Paris VII-CNRS, were held Sept. 5-13, 1985, at Universitaire de Paris, Paris, France. M.J. Hiza, Scientific Program Committee member.

AIChE Meeting sessions on Membrane Separations and Approaches to Teaching New Technologies, held Nov. 10-14, 1985, in Chicago, IL. R.D. Noble, session chairman.

International Symposium on Fluid Flow Measurement, to be held in Washington, DC, Nov. 16-19, 1986 and jointly sponsored by AGA, API, ASME, GPA, GRI, and NBS. N.A. Olien, member of organizing committee.

International Cryogenics Conference to be held Dec. 10-14, 1985, in Calcutta, India. S.K. Sikdar, Steering Committee member.

WORKSHOPS

Hosted a workshop entitled The Cutting Edge: Research and Applications in Chemical Engineering and Chemistry. Attended by 30 area teachers on Jan. 22, 1985, at NBS, Boulder, CO. Sponsored by NBS and The Colorado Alliance for Science. Organized by D.E. Diller, L.L. Sparks, and S.K. Sikdar.

Hosted a short course on Basic Chemical Instrumentation, Jun. 2-20, 1985,at NBS, Boulder, CO. Course was attended by 35 NBS scientists, and students from the University of Colorado and the Colorado School of Mines. Organized and taught by T.J. Bruno.

Hosted a NASA sponsored workshop on Helium Transfer in Space, Aug. 20-21, 1985, at Boulder, CO. Attended by participants from government, universities, and industry from throughout the world. Organized by D.E. Daney and co-directed by V.D. Arp.

Participated in a panel to review, evaluate, and rank research proposals to the National Science Foundation in Washington, DC, Sept. 9-10, 1985. N.A. Olien.

Hosted an international workshop on Two-Phase Flow at NBS-Gaithersburg, sponsored by DOE-Office of Basic Energy Sciences, Sept. 22-27, 1985. Chaired by J. Kestin and organized by G.E. Mattingly and N.A. Olien.

SEMINARS

Dr. Damon Seok, Department of Chemical Engineering, University of Cincinnati, Cincinnati, OH: A New Approach to the Membrane Gas Separation, Nov. 13, 1984.

Dr. Delbert J. Eatough, Thermochemical Institute, Brigham Young University, Provo, UT: Solution Calorimetry and its Applications to the Study of Molecular Interactions in Model Coal Liquids, Nov. 15, 1984.

Professor William B. Krantz, Department of Chemical Engineering, University of Colorado, Boulder, CO: Interfacial Structures Arising from Instabilities Due to Very Large Concentration Gradients, Dec. 7, 1984.

Dr. Stanley Abramowitz, Chemical Thermodynamics Division, NBS/CCP, Gaithersburg, MD: Programs in the NBS Biotechnology Program, Dec. 12, 1984.

Dr. Terry G. Lenz, Department of Agricultural and Chemical Engineering, Colorado State University, Fort Collins, CO: Solar-Thermochemical Energy Conversion Research at CSU, Jan. 10, 1985.

Dr. Mark Donahue, Department of Chemical Engineering, Johns Hopkins University, Baltimore, MD: Thermodynamics of Heavy Hydrocarbons, Jan. 14, 1985.

Ms. Peggy Phillips, Professional Nutrition Services, NBS, Boulder, CO: Everything You Wanted to Know About Vitamins, Jan. 25, 1985.

Dr. James E. Zimmerman, Electromagnetic Technology Division, NBS/CEEE, Boulder, CO: Impressions of China, Feb. 1, 1985.

Mr. Paul Bergstrom, Atlantic Richfield Co., Denver, CO: Hazardous Waste, Feb. 15, 1985.

Dr. John W. Flock, Chemical Engineering Branch, General Electric R&D, Schenectady, NY: Chemical Engineering Research at General Electric Corporate R&D Center, Feb. 20, 1985.

Dr. Larry Belfiori, Colorado State University, Fort Collins, CO: Amorphism in Semicrystalline Polymers via Cryogenic Pulverization, Feb. 21, 1985.

Dr. Richard A. Bartsch, Department of Chemistry, Texas Tech University, Lubbock, TX: Coupled Metal Ion Transport Across Bulk Liquid and Emulsion Membranes by Ionizable Crown Ethers, Mar. 15, 1985.

Professor Maurice Kreevoy, University of Minnesota, Minneapolis, MN: Mechanism of Nitrate Removal from Water by Solid-supported Liquid Membranes, Mar. 20, 1985.

Dr. John D. Lamb, Brigham Young University, Provo, UT: Cation Selectivity of Macrocyclic Ligands in Homogeneous Solution and in Liquid Membranes, Mar. 22, 1985.

Dr. Dale Gillette, National Oceanic and Atmospheric Administration, Boulder, CO: Wind Erosion, Mar. 29, 1985

Professor Donald L. Koch, Chemical Engineering Department, Massachusetts Institute of Technology, Cambridge, MA: Dispersion in Porous Media, Apr. 10, 1985.

Professor T. Alan Hatton, Chemical Engineering Department, Massachusetts Institute of Technology, Cambridge, MA: Biochemical Processing Using Reversed Micelles, Apr. 15, 1985.

Dr. William J. Ward, General Electric R&D, Schenectady, NY: Rayleigh-Benard Convection in Electrochemical Redox Cell, Apr. 22, 1985.

Mr. Donald Hearth, University of Colorado, Boulder, CO: Space Programs in the U.S. - Past, Present, and Future, Apr. 26, 1985.

Dr. Carol McConica, Colorado State University, Fort Collins, CO: Integrated Circuit Processing: A Chemical Engineer's Challenge, May 10, 1985.

Dr. John Wagner, Food, Protein Research and Development Center, Texas A&M, College Station, TX: Overview of Engineering Research Programs on Replenishable Resources at Texas A&M University, Jun. 19, 1985.

Dr. Michael S. Graboski, Syngas Systems, Inc., Golden, CO: Thermal Conversion of Biomass to Gaseous Fuels, Jun. 28, 1985.

Dr. Milan Bier, University of Arizona, Tucson, AZ: Electrophoresis in Biotechnology, Jul. 12, 1985.

Mr. Bob Gates, Public Service Co. of Colorado, Denver, CO: Pollution Control in Power Generation, Sept. 20, 1985.

Ms. Peggy Phillips, Professional Nutrition Services, Boulder, CO: Nutrition for Optimizing Work Performance, Oct. 4, 1985.

Dr. Verle N. Schrodt, Monsanto Co., St. Louis, MO: Research Needs in Separations for Bioprocesses, Oct. 18, 1985.

TECHNICAL ACTIVITIES OF THE THERMOPHYSICS DIVISION (774)

N.A. Olien, Chief

1. INTRODUCTION

The research of the Thermophysics Division focuses on the thermodynamic and kinetic behavior of fluids and solids, with particular emphasis on properties and substances of current importance in chemical engineering.

In order to explore new phenomena, develop highly accurate measurement techniques, provide state-of-the-art data and descriptive theories for broad classes of substances, a three-pronged approach is used. The first prong consists of developing and applying experimental techniques such as acoustical and optical radiation, laser light scattering, magnetic weighing, and rapid measurement methods. The second involves theoretical methods such as thermodynamic theories, molecular theories, microscopic aspects of electrodynamics and hydrodynamics, and nonlinear mathematics. The third prong is computer modeling of microscopic and bulk properties. The focus of these efforts is on: phase-transition behavior; fluid-fluid and fluid-solid interfaces; polydisperse and multiphase fluids; high-temperature solids and liquids; ionic transport and kinetic phenomena such as nucleation. The criteria for the selection of substances and phenomena to be researched are industrial utility, scientific impact, potential for wider applications, and probability of success within given financial and time constraints. The maximum benefits which can be accrued by carefully synthesizing theoretical and experimental input are thoroughly considered in all projects. Modern data processing and electronics, advanced measurement concepts, and new mathematical methods for solving multivariable and nonlinear equations are fully exploited. Current programs include: state-of-the-art thermodynamic properties of substances used in tertiary oil recovery, geothermal energy, synthetic fuels, and supercritical extraction; interfacial wetting; modeling of coal-like solids; polydisperse fluids; and critical-point and fluid-solid phase transformations.

2. GOAL

The goal of the Division is to perform exploratory research on the thermophysics of gases and condensed phases, for the purpose of establishing state-of-the-art measurement procedures, fundamental concepts, basic theories, and predictive models which advance the understanding and applications of thermodynamic and transport properties in chemical engineering.

3. GROUP AND PROGRAM FUNCTIONS

Groups

- Equation of State-Johanna Levelt Sengers, Group Leader

This group performs experimental studies of PVT relationships in fluids, phase equilibria and PVTx relationships in binary and multicomponent fluid mixtures. State-of-the-art measurement techniques are being developed for Burnett-isochoric PVT determinations, light scattering measurements near phase boundaries, magnetic densimetry, PVTx measurements of multiphase equilibria, and critical lines in mixtures. The group also develops thermodynamic models of mixtures and pure fluids which are based on fundamental concepts such as scaling and universality, and which utilize the latest advances in the renormalization group and corrections to scaling; collaborations with members of the Statistical Physics Group exist to model mixtures by means of perturbation theory and theories of polydisperse systems.

- Statistical Physics-John M. Kincaid, Group Leader

This Group conducts theoretical studies of gases and condensed matter in both equilibrium and nonequilibrium states. The methods of statistical mechanics and fluid mechanics are used to formulate theories of: thermophysical properties of solids; transport phenomena; polydisperse mixtures; ion motion in solutions, pores, and membranes; chemical reaction kinetics; radiative cooling; fluctuation phenomena; and dynamic phase transformations and interfaces. These studies make use of a wide range of mathematical and computational techniques. Close ties are maintained with the Equation of State Group and other technical programs in the Division through collaborations, informal discussions, and seminars on topics of mutual interest.

Programs

- Condensed Matter-Raymond D. Mountain, Technical Leader

The objectives of this program are to develop models of phase transitions and of nucleation and growth in metastable fluids; to study spectroscopic probes, such as collision-induced infrared absorption for determining key molecular parameters which characterize bulk properties of fluids; and to explore methods for modeling amorphous solids, such as coal.

o Dynamic Measurements-Ared Cezairliyan, Technical Leader

The purpose of this program is to develop dynamic (millisecond and microsecond resolution) measurement techniques; perform measurements of selected thermophysical properties of high melting point substances to temperatures over the range 1500-10,000 K; develop high temperature Standard Reference Materials; probe nonequilibrium phenomena such as superheating; and investigate high temperature, and high temperature and high pressure (GPa) regions of melting and polymorphic phase transitions. The unique capabilities of this laboratory provide the means to obtain thermophysical data in a temperature regime where conventional techniques fail to operate because of the exposure of the specimen to high temperature for prolonged periods and because of long equilibration times.

o Interfacial Phenomena-Michael R. Moldover, Technical Leader

The purpose of this program is to: (1) experimentally characterize the occurrence, stability, thickness, and transport properties of intruding wetting layers which often form when two fluid phases are in contact with a third phase; (2) check the validity of proposed theories for interfacial wetting; (3) develop the spherical acoustic resonator as a state-of-the-art measurement tool for equilibrium and transport properties of gases and gaseous mixtures; and (4) apply the acoustic resonator to the measurement of the universal gas constant, R, and the thermodynamic temperature of the gallium point.

o Thermodynamic Modeling-Lester Haar, Technical Leader

The purpose of this program is to develop algorithms for correlating and extending thermodynamic property values for widely used fluids such as ammonia, water and steam, and aqueous mixtures. The models incorporate results of microscopic formulations for the Helmholtz free energy and use elaborate statistical methods to treat effects of, for example, nonrandom errors in thermodynamic measurements.

4. SELECTED PROJECT SUMMARIES

Film Balance

G. Morrison, H.A. Davis, I.L. Pegg

During the past year, design and construction of the film balance was completed. The balance is composed of four parts. First is a water trough for containing the films; it is constructed entirely of Teflon and rests on a massive thermostatically controlled brass plate. Second is the sensor, which is constructed from a silicon fiber strain gauge, and there are effectively no "moving parts" in the sensor. The third part is the stepper motor mechanism for changing the surface area accessible to the film. Finally, there is a personal computer which controls the stepper motor, records the response on the strain gauge, and stores the data for future use.

The balance is presently being steam cleaned, a precaution necessary to assure minimal contamination of the films from the Teflon trough itself. The instrument will be calibrated and measurements will be made to study fluid-fluid phase behavior in binary monomolecular films.

Semi-Automated PVT Facility

D. Linsky

The pressure measurement capability has been expanded through the acquisition of a commercial 18 MPa gas-lubricated piston gage. The gage has been cross-calibrated with the 4 MPa piston gage and the existing Bourdon gage, with the latter used in the absolute mode (reference to vacuum). A large amount of software development has been done. BASIC programs for running PVT experiments and for collection and reduction of data have been written, with increased versatility and for different combinations of tasks. Hardware and software development has begun for automated temperature selection and control through the use of a programmable ratio transformer, and for remote monitoring of experimental conditions via telephone lines to distant terminals.

V-L-E FACILITIES

G. Morrison, K.A. Johnson, F. Guzman, H.A. Davis

There is a long term commitment to the development of a variable volume V-L-E cell which does not use mercury and which has the option for sampling. The past year has seen a major redesign of one portion of the cell to allow the cylinder to be honed in the event of severe damage to the cylinder walls. There has also been a small modification to the piston drive screw to keep several closely spaced parts of the drive mechanism from pushing against one another and binding. In addition to the aforementioned changes, the stepper motor and motor driver were replaced and the computer software driving the motor was altered to avoid losing pulse count and to switch off the power to the motor when it was not being powered. At present, the cell can be used in a restricted mode. When a problem with the integrity of the dynamic seal is solved, the cell will be put into full use and the sampling valve will be tested.

During the next year, a methodical study of mixtures of n-alkanes with average chain length of six carbons will be studied. The motivation of this study is to test the model of polydisperse fluid mixtures and to examine how a fluid "senses" its multicomponent nature.

Properties of Refrigerant Mixtures

G. Morrison, D. Didion*, P. Domanski*, M. McLinden*, R. Radermacher*

The major activity of the past year centered around producing a technical note to summarize the results of the previous three years' work on this project. That document is presently in a final draft form and is being typed. In this document, we discuss the application of a modified Carnahan-Starling equation of state to refrigerant mixtures. We also discuss important phase behavior, such as phenomena induced by nearby critical points and the prediction of the temperature and pressure dependence of azeotropes; this discussion is carried out by using specific refrigerant mixtures as examples. In addition, one section of this note covers the generation of thermodynamic functions from equations of state and perfect gas information, definitions of reference states, ideal mixtures, and the connection between real mixtures and pure material reference conditions. The last two sections of the note give data for pure refrigerants and some of their mixtures, and a complete listing of the computer codes for calculating the phase diagrams and thermodynamic properties of refrigerants.

The second activity connected with this project has been one of technology transfer. Modeling refrigerant mixtures with a modified Carnahan-Starling equation of state has been discussed in papers given at ASHRAE (American Society of Heating, Refrigerating, and Air-conditioning Engineers) meetings in Chicago (January, 1985) and Honolulu (June, 1985). It was also discussed at a Workshop on the Application on Nonazeotropic Refrigerant Mixtures sponsored by EPRI (Electric Power Research Institute) and hosted by Hawaiian Electric.

*NBS Center for Building Technology (NBS Division 745)

Working Fluid Mixture for Binary Geothermal Power Cycle

P. Albright, J.S. Gallagher, J.M.H. Levelt Sengers,
D. Linsky, G. Morrison, M. Emeruwa

The experimental VLE and PVT work on a 90%-10% mixture of isobutane and isopentane, a working fluid for the geothermal Heber plant is being completed. A supercritical reference PV isotherm has been established by means of six Burnett runs and measurements are then made along isochores intersecting this isotherm. VLE measurements have been taken in the range of 50-90 ^{o}C. The thermodynamic surface for this mixture is in a final round of refinement, and estimates have been made of the effect of the most prevalent impurity, n-butane. Two papers on this work were presented at the Ninth Symposium on Thermophysical Properties at Boulder, June 85, and a M.Sc. thesis resulted from it. A new attempt is being made at a scaled formulation of the region near the critical line.

Rayleigh Light Scattering from Near-Critical Fluid Mixtures

R.F. Chang

We have completed a systematic experimental investigation of the critical dynamics of mixtures of carbon dioxide and ethane near the vapor-liquid critical line. Measurements have been made of the decay rate of critical fluctuations for three compositions of the mixtures as well as pure carbon dioxide and ethane. The compositions of the mixtures are 0.054, 0.358, and 0.680 mole fraction of carbon dioxide with the last composition being near-azeotropic. Our data indicate that the mixtures exhibit cross-over behavior from pure fluid-like to mixture-like as a critical point is approached although there is only one dominant mode of fluctuations at all times. Consequently, the order parameter also crosses over from density (heat mode) to concentration (mutual diffusion mode) while this mode of fluctuations is still governed by the mode coupling theory regardless of the nature of the order parameter. The results of the investigation have been presented in a paper entitled "Decay Rate of Critical Fluctuations in Ethane+Carbon Dioxide Mixtures near the Critical Line Including the Critical Azeotrope" at the Ninth Symposium on Thermophysical Properties (Boulder, CO, June 24-27, 1985) and are to be published in the International Journal of Thermophysics.

Crossover

P.C. Albright

The term "crossover" refers to the transition from classical to nonclassical behavior that most systems make when they approach their critical point. Since remnants of the critical behavior can often still be seen far from the critical point, an understanding of the crossover behavior is important in the reliable formulation of thermodynamic surfaces, as well as in the understanding of thermodynamic processes designed to operate near the critical region.

In collaboration with J.V. Sengers and J. Chen of the University of Maryland, we have developed a primitive implementation of the theoretical crossover theory for the liquid-vapor critical point. The model seems to already be superior to the most sophisticated techniques currently used for describing the critical region. The basic theoretical notions were presented at the Ninth Symposium on Thermophysical Properties in Boulder, June 1985, and are being published in the proceedings. Refinements of the model are currently being tested. These refinements include considering the lowest-order asymmetries known to be important in real fluids, and matching the generic mean-field regime with an appropriate noncritical (e.g. virial) equation of state.

A further extension of the above work is in the development of a crossover theory for fluid mixtures. The theoretical work has been essentially completed; we will implement the theory when we have gained some more experience with the pure fluid case.

In collaboration with J. Nicoll, J.V. Sengers, and J. Chen, we are engaged in extending the earlier work to a crossover theory of the k-dependent correlation function. This will constitute the Ph.D. thesis of Mr. Chen. This collaboration has so far resulted in some modest improvement of extant asymptotic theories.

Further theoretical work includes calculation of crossover equations of state within the context of the renormalization group theory. Results from these calculations have been published, or are currently in the review process, and include new calculations of asymptotic amplitude ratios (both leading and correction-to-scaling), calculation and analysis of asymptotic parametric equations of state, and an analysis of the region of validity of the Wigner series.

(Dilute) Near-Critical Mixtures and Aqueous Electrolyte Solutions

R.F. Chang, C.M. Everhart, J.M.H. Levelt Sengers, G. Morrison, G. Nielson

Near-critical fluid mixtures, especially when they are dilute, display large anomalies in thermodynamic behavior. An appreciation of these effects is important to the understanding of impurity effects in custody transfer and in working fluids for supercritical Rankine cycles, to the understanding of supercritical solubility, and to the understanding of the very large anomalies found in near-critical aqueous electrolyte solutions.

At the AIChE Symposium on Supercritical Fluids, San Francisco, November 1984, we presented a detailed explanation of the supercritical heat-of-mixing effects reported by Christensen et al. With K.S. Pitzer, we are working on describing the anomalous partial molar properties of near-critical aqueous electrolyte solutions. We reported this work at the Houston AIChE meeting (March 85), and by a poster at the NBS Electrolyte Workshop in June 85; we also submitted a paper for publication to Chemical Engineering Communications.

One of us (G.N.) has developed a model for supercritical solubility that maps the properties of the dilute solution onto those of the pure solvent. Another (G.M.) has classified the supercritical solubility effects in their dependence on number of components and number of phases present, and corrected or explicated several ambiguous statements in the literature. Our work was presented in papers at the Ninth Symposium on Thermophysical Properties in Boulder, June 1985, and at the April 1985 ACS meeting at Miami Beach.

Dimensionless Formulation of Thermophysical Properties of H_2O and D_2O

J.S. Gallagher, J.V. Sengers

The dimensionless forms of the Haar-Gallagher-Kell (HGK) formulation for H_2O and the Hill-McMillan formulation for D_2, along with scaling law representations of these two substances for use in the critical region, have been assembled onto a computer tape. This tape will be distributed by the Office of Standard Reference Data as a "Standard Reference Database." These programs will allow the user to interactively calculate thermodynamic and transport properties of these two substances, using a system of units chosen by the user and with a variety of property pairs as independent variables.

Droplet Growth in Mists

G. Morrison, J. Kincaid, R.F. Chang

We are planning to study the time development of the particle size distribution of a mist formed from a multicomponent, initially binary, liquid mixture. Since settling of the mist is a serious problem (for the long-time behavior) that interests us, we anticipate that the experiment will ultimately be carried out in a microgravity environment. This project is being supported by NASA. Our motivation is to study the effect of the multicomponent character of the mixture on the evolution of the droplet size distribution, and the possibility of long-time quasi-equilibrium states. A number of exploratory experiments will first be performed on earth. We are presently concerned with the method of generating the mist, its characterization on earth, and the evaluation of suitable techniques for a microgravity experiment. We expect to generate the mist ultrasonically using piezoelectric transducers. Detailed size distribution of the mist can be obtained from laser Doppler velocimetry of the particles in free-fall. To determine the potential of different measurement techniques for the microgravity experiment, we will evaluate direct microscopic photography, Brownian diffusion, and holography using systems of particles of known size (and size distribution) suspended in a density matched medium.

Phase Behavior of Supercritical Polymeric Solutions

E.J. Clark, J.M.H. Levelt Sengers, P.H.E. Meijer*

Supercritical solvents have significant potential application in the extraction and separation of organic materials which require high temperatures for conventional processing methods, and yet are degraded by the same elevated temperatures. Polymer processing is an example. A data base of appropriate references in the field of polymers and supercritical extraction has been started. We propose to study the phase behavior of polyethylene in supercritical solutions. From the very few studies that have appeared in the open literature, it has been found that the phase diagrams are fairly complicated, with liquid-liquid phase separation occurring near the solvent's vapor pressure curve in the P-T plane. The region of phase separation can be moved to lower temperatures by the use of a second, supercritical solvent. Initial experiments will include the study of polyethylene solubility and crystallization in supercritical one-component solvents by means of a simple visual cell. The location of phase boundaries will be assessed by varying the temperature and/or pressure. A theoretical effort to model these phase diagrams and predict the solubility of polymers in supercritical fluids will be carried out in parallel to the experimental studies.

*Catholic University

Molecular Dynamics Studies of Fluid Mixtures

R.D. Mountain, G. Birnbaum (NBS Division 401)

The method of molecular dynamics simulation is being used to investigate the dynamical processes involved in the phenomenon of collision-induced absorption of far infrared radiation in rare gas mixtures. Our work on Ar-Ne and Ar-Kr mixtures strongly suggests that intrinsic three-body interactions are observed in this process. A simulation of the parahydrogen-helium system has been made, as this is the simplest system for which ab initio quantum mechanical calculations of the interactions and induced moments can be made. The results of this study will be used to guide the quantum mechanical calculations being made elsewhere.

Molecular Dynamics Study of a Model Reference System for a Biological Membrane

R.D. Mountain, R. Mazo (University of Oregon)

A set of molecular dynamics simulations were made, on a simple two-component mixture of strongly repelling disks, in order to provide a reference system for a lipid-protein membrane. Measurements of the lipid-protein interaction, using spin-resonance techniques, require a knowledge of the fraction of lipid molecules which are "next to" one or more of the protein molecules in the membrane. This is a manifestation of the three-body-correlation problem which is not amenable to analytical solution. The simulation results provide a direct resolution of this question and will provide the basis for refined interpretation of biophysical measurements.

Relative Stability of Dense Random Packings

R.D. Mountain, H.J. Raveche

An extensive molecular dynamics investigation has been made of the relative stability of fcc, hcp, and random close packings for crystals composed of particles interacting via the inverse-twelfth power of particle separation. No significant difference in the P-T relation for systems of 576 and 4608 particles were found for the different structures. These results will serve as a stringent test for statistical mechanical theories of crystallization.

Thermal Properties of Solid Gas Hydrates

R.D. Mountain, R.A. MacDonald

This is a collaborative effort with Jane Callanan in Boulder (NBS/CCE, Division 773) and M.L. Klein of the National Research Council of Canada. It is partially supported by DOE. A new NBS CYBER 205 code has been written and tested using the molecular model we developed last year. We are now in a position to begin investigating the stability of these structures.

Kinetic Simulation of Aggregation of Particulates

R.D. Mountain, F.E. Sullivan (NBS Division 713),
G.W. Mulholland (NBS Division 753)

The kinetics of the growth of particulates undergoing Brownian motion and aggregation is being studied by means of computer simulation using the "Brownian dynamics" method. Results have been obtained for the free molecular regime and for the continuum limit for the background gas. In the course of this work, a very efficient simulation code was developed. Copies of this code have been provided to researchers at the University of Maryland and at the Desert Research Institute, Reno, Nevada. Two research papers have been written describing the results and the code used to obtain the results.

Thermal Properties of Coal

R.A. MacDonald, R.D. Mountain, J.E. Callanan (NBS Division 773)

The theoretical work on coal has taken two rather different approaches. One, the kinetic model of Merrick, relates the heat capacity to the loss of volatile matter from the coal. The other sets up a 'gel' model to represent a porous, disordered structure, such as coal, and calculates the properties of this structure.

We find that Merrick's model gives a satisfactory representation of the heat capacity results for coal specimens sealed in various atmospheres (air, nitrogen, carbon monoxide, argon, and helium). The model, as it stands, cannot account for the behavior (mainly exothermic) observed on initial heating of the specimens, nor can it explain the role played by the atmosphere in these initial runs. We conclude that, while the initial run effects are not pertinent to realizing the true heat capacity of the coal, they nevertheless contribute significantly to the heat balance of systems utilizing raw coal and, for this reason, warrant further study. These results were presented at the Ninth Symposium on Thermophysical Properties, Boulder, June, 1985, and will be published in the International Journal of Thermophysics. The experimental part of this work has been carried out by J.E. Callanan and S.A. Sullivan of the Center's Chemical Engineering Science Division.

The 'gel' model has as its basis a hexagonal close packed lattice, containing 1200 atom sites. The gel is generated by a random procedure of bond selection, the disorder being represented by missing bonds and missing atoms. We have used the equation-of-motion method to calculate the frequency spectrum for several particle densities. We find that the disorder has a marked effect on the frequency spectrum, shifting a large number of modes from high to low frequencies. Also, when in-plane to out-of-plane bond strengths are in the ratio 2:1, there is a further shift to lower frequencies and the two-peaked spectrum expected for an anisotropic structure develops. We conclude that the gel model provides a satisfactory basis for development as a model of coal. This work was presented at the Ninth Symposium on Thermophysical Properties, Boulder, June 1985, and has been accepted for publication in the International Journal of Thermophysics.

Equilibrium Properties of Polydisperse Fluids

K. Johnson, D. Jonah, J. Kincaid, G. Morrison, D. Tsai

The objectives of this work are to investigate polydisperse models for the thermodynamic properties of multicomponent fluids, and to develop accurate methods for determining the properties of real polydisperse systems, such as petroleum. Equations of state and phase equilibria play an essential role in the separation processes used by the chemical process industry. This work will provide simple, accurate methods for measuring, as well as modeling, important characteristics of phase equilibria and thereby provide industry with the means to substantially increase the efficiency of separation processes.

We continue to elucidate the relationship between polydisperse systems and systems with a finite number of components. An elegant functional analysis of the critical conditions of model polydisperse fluids was published in the Journal of Chemical Physics. We showed that the critical-point conditions can be expressed in terms of two Fredholm determinants, the calculus of which demonstrates that the critical conditions may be viewed as a well-controlled limit of the corresponding finite-component conditions.

In a paper submitted to the AIChE Journal, we presented a novel expression for the Gibbs free energy of a very dilute binary mixture, the input to which depends primarily on measured thermodynamic properties of the pure solvent. This has been successfully applied to the correlation (and prediction) of data on gas solubilities in liquids, supercritical fluid extraction, and vapor-liquid equilibria at ordinary temperatures and pressures.

Both of these topics were presented at the Ninth Symposium on Thermophysical Properties, Boulder, June 1985.

Inhomogeneous Reaction Kinetics

J.B. Hubbard, J. Mercer, F. Martinez

This project provides the essential theoretical modeling for chemical reaction kinetics in situations where large concentration gradients exist. Examples are pulse radiolysis, ultrasonic chemistry via acoustic cavitation, and plasma recombination. While a detailed quantitative description of these processes is far beyond our present capabilities or needs, it is highly desirable to have a relatively simple phenomenological model of considerable generality which allows thorough mathematical analysis. Our approach to this problem is as follows: Imagine the sudden creation of a concentrated "pulse" of reactants in an infinite "condensed" medium, and the subsequent competition between a variety of irreversible recombination reactions and Fickian mass diffusion. How does the total number of particles (free radicals for instance) of a given species at a given time depend on the shape of the initial pulse, the diffusion coefficients, rate constants, order of the reactions, and the dimensionality of space? In particular, how does the survival fraction at infinite time depend on these parameters?

We restricted ourselves to a single species with an initial Gaussian profile, to reaction kinetics of second, third, and fourth order, and to one, two, and three spatial dimensions. We then performed a thorough numerical investigation of the solutions to these nonlinear partial differential equations; in addition, we utilized and developed a variety of analytic methods to obtain physical insight as well as approximate solutions. These include rigorous upper and lower bounds on the survival fraction via functional analysis, Padé approximation techniques, and a "prescribed diffusion" or Gaussian approximation. Our analytical results agree quite well with our numerical work, which requires large amounts of computer time for accurate predictions.

As might be expected, homogeneous reaction kinetics are never attained, even at infinite time; however, the "yield" or survival fraction can be calculated very accurately from our low order polynomial fitting functions of a single dimensionless parameter.

Theories of Solvated Ion Dynamics

J.B. Hubbard, P.G. Wolynes*

We have recently completed a 150-page monograph on the dynamical behavior of solvated ions in polar fluids. This will appear as a chapter in the book The Chemical Physics of Solvation, which is part of a series devoted to modern developments in electrochemistry.

*University of Illinois

Hydrodynamics of Magnetic and Dielectric Colloidal Dispersions

J.B. Hubbard, P. Stiles*

A paper on this subject has been prepared for the Journal of Chemical Physics. In it we develop a theory for the hydrodynamic behavior of colloidal suspensions, the particles of which possess electric or magnetic moments. Particular attention is given to the case where an external electric or magnetic field acts on a system in which the polarization does not relax instantaneously, so that reorientational Brownian motion is coupled to both the field and to hydrodynamic degrees of freedom. Magnetosonic and magnetoviscous effects are derived, with emphasis on anisotropy with respect to the external field.

*MacQuarrie University, Australia

Computer Simulations of Dipolar Molecules Near Neutral and Charged Hard Walls and Simulations of Ionic Mobility in a Polar Fluid

J.B. Hubbard, J. Rasaiah, S. Lee

We are in the middle of a molecular dynamics simulation of a Stockmayer fluid between two impenetrable plates which may be electrically neutral or charged. We are interested in obtaining the equilibrium wall-molecule "density" distribution function, as well as the polarization profile. We also plan to extract the single particle diffusion coefficient normal and parallel to the walls.

We designed the ion mobility molecular dynamics simulation to test current theories as well as provide valuable information on solvated ion dynamics in bulk media. We are particularly interested in seeing how well the statistically averaged time integral of the ion's velocity autocorrelation function agrees with the averaged time integral of the force autocorrelation function for a "fixed" or immobile ion. This is the Brownian dynamics ansatz, which is strictly valid only for infinitely massive ions, but which is a key assumption in all current theories of ion motion in fluids.

Computer Simulations and Theory of Diffusion Controlled Reaction Kinetics in the Presence of Density and Composition Fluctuations

J.B. Hubbard, J. Rasaiah, S. Lee, R. Rubin (NBS Division 440)

This project was conceived in order to investigate the importance of fluctuations in diffusion controlled reactions. It has recently been established that composition fluctuations can exert a profound influence on annihilation reactions of the class A+B inert. In this instance, with equal numbers of the two species and an initial spatially uniform A-B distribution, it can be shown that the concentration decays as $t^{-d/4}$ ($d \leq 4$) at long times, where d is the spatial dimension. This is in stark contrast to the prediction of homogeneous reaction kinetics, which yields a t^{-1} law for the concentration decay. The reason for this breakdown is that small concentration fluctuations, which are the inevitable consequence of thermally driven molecular motions, become more significant as the reaction progresses, and actually dominate the kinetics at long times. We are currently investigating other systems which might exhibit similar behavior by means of a "lattice random walk/cellular automata simulations" of diffusion and annihilation. We have already established that in the reaction A+A-->inert, the long time behavior of the system is completely independent of the initial configuration, which implies that future simulations might be streamlined by selecting optimal conditions for statistical processing.

Among the systems we plan to investigate (in 1-3 dimensions) is the parallel reaction A+A-->inert/A+A*-->inert, where A* refers to a trapped or immobilized molecule, and for which the trapping event itself is modelled as a stochastic process.

Conference on Electrolyte Solutions

J.B. Hubbard, J. Rasaiah

A conference on electrolyte solutions in science and engineering was held June 10-12, 1985, at NBS in Gaithersburg, MD. Approximately 50 participants and 12 speakers from five countries discussed topics ranging from statistical mechanical theories of electrolyte solutions, to processes at semiconductor electrodes, to recent advances in fuel cell technology. A poster session was also provided to facilitate the rapid, informal exchange of ideas. The casual atmosphere, combined with the rather diverse interests of the attendees, provided an environment that encouraged many thoughtful and lively discussions.

International Formulation of Thermophysical Properties of Light and Heavy Water and Steam

J.V. Sengers, J. Kestin

The International Association for the Properties of Steam (IAPS) adopted the formulations of the thermodynamic properties of H_2O and D_2O at the Moscow meeting, September 1984 and authorized J.V. Sengers to prepare the releases. These were written and circulated among all member countries by the end of 1984. After receiving input from some of the members, these releases were finalized. We wrote an article about these releases for the Journal of Physical and Chemical Reference Data. During the past year a draft release was also prepared for the thermal conductivity and viscosity of H_2O. This release was adopted, subject to editorial changes, at the IAPS Executive meeting, NBS, Gaithersburg, MD, September, 1985. At this Executive meeting, J.V. Sengers was authorized to prepare, in collaboration with W. Wagner (Bochum, W. Germany), a release on coexistence properties of steam. With J. Nieuwoudt, an article was submitted to Physica on the viscosity of mixtures of H_2O and D_2O.

IUPAC Book on Ethylene

J.V. Sengers, R.D. McCarty (Division 773), J.M.H. Levelt Sengers, R. Jacobsen*, H.J. White, Jr.**

IUPAC is planning to publish a book on the thermodynamic properties of ethylene. It will be based on the work sponsored by the consortium organized by the Office of Standard Reference Data (OSRD) in the 70's. At a meeting held at the time of the Ninth Symposium on Thermophysical Properties in Boulder, June 85, an agreement was reached on the content of the book, and writers were appointed for the various chapters. The plan is to have a draft completed by the end of 1985.

* University of Idaho
**NBS Office of Standard Reference Data

Thermophysical Measurements in Microgravity Environment

A. Cezairliyan, A.P. Miiller, M.S. Morse

A system was constructed for the dynamic measurement of heat capacity and electrical resistivity of high-temperature liquid metals above 2000 K in a microgravity environment. This system is an extension of the unique millisecond-resolution facility developed earlier in this laboratory for the dynamic measurements of selected thermophysical properties of solids at high temperatures. This new development permits extension of the accurate measurements to temperatures above the melting point of the specimen and possibly several thousand degrees into the liquid phase. As a part of the initial phase of this program, modifications were made to the system and a new series of pulse experiments in a microgravity environment (KC-135 aircraft flights operated by NASA in Houston) were performed during May 1985. The objectives were to study the geometrical stability of the specimen (liquid niobium rod) during rapid melting experiments, and obtain data on mechanical vibrations which may be affecting the stability of molten specimens. The experiments on board the KC-135 aircraft were conducted by P. Giarratano of the Center for Chemical Engineering in Boulder. The results of a total of 30 experiments indicated that the specimens retained their geometry for a brief period after melting and confirmed the reproducibility of the measurements. Also the accelerometer data suggest that aircraft vibrations are transferred to the molten specimen affecting its stability. Changes and refinements in the system are underway to further improve operation of the system. Plans were also made for the extension of this program to perform experiments aboard the Space Shuttle in about 3 years.

Microsecond-Resolution Thermophysical Measurements

A. Cezairliyan, J.L. McClure, M.S. Morse

Development of an ultra-fast technique for the measurement of thermal properties (heat capacity, electrical resistivity, heat of fusion, etc.) of very high temperature (2,000-10,000 K) materials is under way. This will enable extension of the present capabilities to specimen heating rates about 1000 times greater than achieved before in our laboratory, and to measurements on high temperature liquid conductors. During the present year, development and testing of a new accurate technique for measuring electrical quantities in capacitor discharge experiments has been completed. As a result, we are able to measure high pulse currents (50 kA) and high pulse voltage (20 kV) at one MHz rate with an uncertainty of less than 1%. This complements the fast temperature measurement capability developed earlier in our laboratory. During 1986, the system will be used to measure heat of fusion of a refractory metal, such as niobium. This technique is likely to provide heat of fusion data on refractory metals with an accuracy never attained before.

Properties of Graphite

A. Cezairliyan, A.P. Miiller

In recent years, graphite has become one of the most important refractory materials in the development of high-temperature technologies, finding applications as a thermal protective material, as a component in structural composites, etc. It also has the potential of becoming a reference material for thermal property measurements. As a result, there has been increasing need for accurate data on various thermophysical properties of graphite, particularly at temperatures above 2000 K, where significant disagreements exist in the literature.

In our laboratory, two studies related to graphite are under way: (1) measurements of the heat capacity and electrical resistivity above 1500 K, and (2) measurement of the triple point temperature.

(1) During FY 85, accurate measurements of the heat capacity and electrical resistivity of POCO AXM-501 graphite were conducted in the temperature range 1500-3000 K as part of the CODATA program on properties of high-temperature reference materials.

(2) Preliminary measurements of the triple point temperature of graphite have been performed. The measurements were conducted with the specimen in a pressurized gas environment at about 14 MPa. Temperature measurements were made with a newly constructed pyrometer which measures spectral radiance temperatures at six wavebands. The final measurements will be made in 1986 after completion of the final testing and calibration of the pyrometer. The estimated uncertainty of the triple point temperature measurements is about 50 K. Data reported in the literature range from 3900-5000 K.

Shear Viscosity

R. Berg, M.R. Moldover

A torsion oscillator has been developed to measure the viscosity of fluids at moderate temperatures (-100 ^{o}C to + 100 ^{o}C) and pressures (0-10 MPa) at very low frequencies (0.5 Hz) and very low shear rates (0.05 s^{-1}). The oscillator will be used in a NASA sponsored project for testing the theory of dynamic critical phenomena. This viscometer is now being used to study microemulsions and alkali metal mixtures.

Optical Studies of Interfaces

R.F. Kayser, M.R. Moldover, J.W. Schmidt

We have used ellipsometry to measure the thickness of wetting layers of SF_6 on a vertical, fused silica surface. The thickness decreases from 40 to 20 nm as the height of the measurement (above a liquid-vapor meniscus) is increased from 1 to 4 mm. In equilibrium, the thickness of the wetting layer is determined by the competition between gravitational forces tending to thin the layer and the long-range part of the intermolecular force between SF_6 and silica. Our data are consistent with the Dzyaloshinskii-Lifshitz-Pitaevskii theory of dispersion forces. We are now studying the drastic changes in the thickness of wetting layers caused by temperature gradients. Our measurement techniques are applicable to other transparent fluids such as CO_2, hydrocarbons, and brines which are encountered in petroleum reservoirs.

The theory of universality of critical phenomena has been used to relate the interfacial tension in the critical region of many fluids to any of three other quantities: (1) the correlation length as measured by light scattering, (2) the anomalous part of the equation of state, and (3) the anomalous part of the heat capacity. The theoretically based relations for correlating interfacial tension appear to be useful at liquid-vapor critical points, consolute points of ordinary solutions, and consolute points of polymer solutions. Experiments to further test this theory have recently been completed in binary liquid mixtures near upper consolute points and lower consolute points.

During the past year, this work has led to invitations to speak at two Gordon conferences, a symposium of the Faraday Society, topical meetings at College de France and Brookhaven National Laboratory, and several colloquia at universities.

Spherical Acoustic Resonators for Thermophysical Properties and Standards Measurements

T.J. Edwards, M.R. Moldover, J.P.M. Trusler

New stainless steel and quartz acoustic transducers are being developed for compatibility with the ultrapure gases required for metrology. The transducers must tolerate a high bakeout temperature; thus, the transducer technology will also be useful for the measurement of the thermophysical properties of technologically important gases at high temperatures.

Two stainless steel spherical acoustic resonators and associated apparatus have been assembled to measure the universal gas constant, R, with the highest possible accuracy. An improvement by a factor of 5-10 over previous measurements is anticipated. The volume of one resonator was calibrated to one part in one million. A gas handling system was assembled and tested. Isotopically enriched argon-40 was obtained from the Mound Laboratory.

A definitive paper entitled "Spherical Acoustic Resonators: Theory and Experiment" was accepted for publication in the Journal of the Acoustical Society of America. Work will continue on this project in 1986.

Phase Equilibrium in the Critical Region of Mixtures

J.C. Rainwater (Division 773), M.R. Moldover

In previous work this project has developed and tested a physically based thermodynamic model for correlating VLE data near the critical locus of binary mixtures. This model has now been codified into a user friendly package suitable for implementation on microcomputers. A recent application of this package used the critical locus data obtained by J.L. Sengers for isobutane-isopentane mixtures to predict the properties of the coexisting phases from the critical locus to half the critical pressure. At these low pressures, our model is in good agreement with VLE predicted by conventional equation of state methods. Near the critical locus, where conventional methods are poor, our model fit the data within their accuracy.

Thermodynamic Modeling of Binary Mixtures

L. Haar, J.S.Gallagher

In the first phase of this program, molecular modeling was applied to the mixture of water with carbon dioxide. A thermodynamic representation was obtained as an expansion about the molecular model, where the expansion terms become negligibly small at high density and/or high temperature. A considerable body of data exists for this mixture. Unfortunately many are clearly inconsistent. It is important to the success of the correlation to ferret out the inconsistent data before global fits are made. To this end, we have employed the molecular model to obtain values of the molecular parameter corresponding to each of the data sets and compared them with literature values. We expect to complete a report containing the thermodynamic surface for the mixture during 1986.

5. HONORS AND AWARDS

J.M.H. Levelt Sengers - Cooperative Interagency Committee on Women in Science and Engineering (WISE) Award for 1985.

G. Morrison and J. Kincaid - NBS Center for Chemical Engineering Outstanding Technical Achievement Award for their research paper entitled Critical Point Measurements on Nearly Polydisperse Fluids.

6. PUBLICATIONS

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Berg, R.F. and Moldover, M.R., Viscosity measurements near critical points using a novel torsion oscillator, Int. J. Thermophysics (Submitted).

Chang, R.F., Doiron, T. and Pegg, I.L., Decay rate of critical fluctuations in ethane + carbon dioxide mixtures near the critical line including the critical azeotrope, Int. J. Thermophysics (Submitted).

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MacDonald, R.A. and Mountain, R.D., A "Gel" model for coal, Proc. of Ninth Symp. on Thermophysical Properties, Boulder, CO, June 1985, Int. J. Thermophysics (Submitted).

MacDonald, R.A., Callanan, J.E. and Sullivan, S.A., Effect of water loss on the heat capacity of coal, High Temperatures--High Pressures, Pion Press, U.K. (Submitted).

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Moldover, M.R., Opportunities for low gravity experiments in critical phenomena, Proc. of NSF Workshop on Opportunities for Academic Research in a Low Gravity Environment (Submitted).

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Nicoll, J.F. and Albright, P.C., Background fluctuations and Wegner corrections, Phys. Rev. B (Submitted).

Sengers, J.M.H. Levelt, Chang, R.F. and Morrison, G., Nonclassical description of (dilute) near-critical mixtures, Symposium Proc. in ACS Series, ACS, April 1985 (Submitted).

Sengers, J.M.H. Levelt, Everhart, C.M., Morrison, G. and Pitzer, K.S., Thermodynamic anomalies in near-critical aqueous NaCl solutions, Chem. Eng. Communic. (Submitted).

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Sullivan, F. and Mountain, R.D., An efficient algorithm for the Brownian dynamics simulation of aggregation, J. Compt. Phys. (In press).

Sullivan, F., Mountain, R.D. and O'Connell, J., Molecular dynamics on vector computers, J. Compt. Phys. (In Press).

Trevino, S.F. and Tsai, D.H., Simulation of the intiation of detonation in an energetic molecular crystal: The overdriven case, Proc. of Eighth Symp. (Int.) on Detonation, July 15-19, 1985, Albuquerque, NM (Submitted).

Wheeler, J.C., Morrison, G. and Chang, R.F., A thermodynamic paradox associated with nonchemical critical phenomena in mixtures, J. Chem. Phys. (Submitted).

7. TALKS

Moldover, M.R., Interfacial Tension of Fluids Near Critical Points and Two-Scaled-Factor Universality, Institute for Physical Science and Technology, University of Maryland, College Park, MD, Oct. 2, 1984.

Moldover, M.R., Optical Studies of Interface Phase Transitions, Physics Department, Lehigh University, Bethlehem, PA, Oct. 11, 1984.

Chang, R.F., Applications of the Leung-Griffiths Model of Mixtures to Dilute Solvents, NBS/CCE Workshop on Supercritical Solvents, Gaithersburg, MD, Oct. 17, 1984.

Mountain, R.D., Kinetics of Particulate Growth via Stochastic Computer Simulation, Colloquium, Physics Department, University of Delaware, Newark, DE, Oct. 24, 1984.

Mountain, R.D., A (Somewhat) New Look at Ultrasonic Scattering for NDE, NDE Panel Presentation, NBS, Gaithersburg, MD, Oct. 31, 1984.

Sengers, J.M.H.L., Thermodynamic Anomalies in Supercritical Fluids Mixtures, Symposium on Fundamental Thermodynamics of Supercritical Extraction, AIChE Annual Meeting, San Francisco, CA, Nov. 26, 1984.

MacDonald, R.A., Thermodynamic Properties of Cubic Metals, Physics Colloquium, Catholic University, Washington, DC, Nov. 29, 1984.

Moldover, M.R., Wetting, Multilayer Adsorption, and Interface Phase Transitions, Chemistry Department Colloquium, University of California, Los Angeles, CA, Dec. 3, 1984.

Moldover, M.R., Wetting, Multilayer Adsorption, and Interface Phase Transitions, Physics Department, University of California, Santa Barbara, CA, Dec. 4, 1984.

Moldover, M.R., Application of Spherical Acoustic Resonators to Measurement of the Universal Gas Constant (R), the Thermodynamic Temperature, and Thermophysical Properties, Solid State Physics Seminar, Physics Department, University of California, Los Angeles, CA, Dec. 5, 1984.

Kayser, R.F., Wetting Layers and Dispersion Forces Between SF_6 and Fused Silica, 52nd Statistical Mechanics Meeting, Rutgers University, New Brunswick, NJ, Dec. 14, 1984.

Kayser, R.F., Wetting Layers and Dispersion Forces Between SF_6 and Fused Silica, Thermophysics Division Colloquium, NBS\CCE, Gaithersburg, MD, Dec. 20, 1984.

Kincaid, J.M., Phase Equilibrium in Continuous Mixtures, Chem. Eng. Dept., University of Virginia, Charlottesville, VA, Jan. 4, 1985.

Moldover, M.R., Wetting, Multilayer Adsorption and Interface Phase Transitions, Physics Department, Pennsylvania State University, University Park, PA, Jan. 22, 1985.

Albright, P.C., A Crossover Theory for Fluids, Washington Area Statistical Physics Symposium, NBS, Gaithersburg, MD, Mar. 20, 1985.

Cezairliyan, A., High-Speed Measurements of Thermophysical Properties at Temperature Above 1500 K, Mechanical and Aerospace Engineering Seminar, University of Delaware, Newark, DE, Mar. 22, 1985.

Sengers, J.M.H.L., Near-Critical Aqueous Salt Solutions, Symposium on Thermodynamic and Transport Properties, AIChE Spring Meeting, Houston, TX, Mar. 25, 1985.

Moldover, M.R. (Coauthors: Kopelman, R.B. and Gammon, R.W.), Turbidity Very Near the Critical Point of Methanol-Cyclohexane Mixtures, American Physical Society, Baltimore, MD, Mar. 27, 1985.

Kayser, R.F., Wetting Layers and Dispersion Forces between SF_6 and Fused Silica, American Physical Society, Baltimore, MD, Mar. 28, 1985.

Kincaid, J.M., Phase Equilibrium in Continuous Mixtures, Chem. Eng. Dept., University of Massachusetts, Amherst, MA, Apr. 1, 1985.

MacDonald, R.A., Thermodynamic Properties of Cubic Metals, Physics Colloquium, Dickinson College, Carlisle, PA, Apr. 15, 1985.

Chang, R.F, Behavior of Dilute Mixtures near the Solvent's Critical Point, APS Spring Meeting, Crystal City, VA, Apr. 24, 1985.

Mountain, R.D. (Coauthor: Mulholland, G.), Simulation of Soot Aggregation, Center for Fire Research Seminar, NBS, Gaithersburg, MD, Apr. 29, 1985.

Sengers, J.M.H.L., Nonclassical Description of (Dilute) Near-Critical Mixtures, Symposium on Equation of State - Theories and Applications, ACS National Meeting, Miami Beach, FL, Apr. 30, 1985.

Moldover, M.R., Wetting Layers and Wetting Phase Transition, Division of Chemical Physics, Chemical Society of France, College de France, Paris, France, May 29, 1985.

Sengers, J.M.H.L. (Coauthor: Everhart, C.), Near-Critical Aqueous Salt Solutions, NBS/CCE Conference on Electrolyte Solutions in Science and Engineering, NBS, Gaithersburg, MD, June 10, 1985.

Sengers, J.M.H.L., Supercritical Solubility, Dept. of Chemical Engineering, University of Maryland, College Park, MD, June 16, 1985.

Kincaid, J.M. (Coauthor: Erpenbeck, J.J.), Calculation of the Mutual Diffusion Coefficient by Equilibrium and Nonequilibrium Molecular Dynamics, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Kincaid, J.M. (Coauthor: Jonah, D.A.), Consideration of Some Dilute Solution Phenomena Based on an Expression for the Gibbs Free Energy, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Chang, R.F., Decay Rate of Critical Fluctuations in Ethane+Carbon Dioxide Mixtures near the Critical Line Including the Critical Azeotrope, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Miiller, A.P., Thermal Expansion of Molybdenum in the Range 1500-2800K by a Transient Interferometric Technique, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Cezairliyan, A., Normal Spectral Emissivity (in the Range 0.5-0.9 Micrometer) of Niobium at Its Melting Point by a Pulse Heating Technique, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 24, 1985.

Sengers, J.M.H.L., Thermodynamic Behavior of Supercritical Fluid Mixtures, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Johnson, K.A. (Coauthor: Kincaid, J.M.), The Critical Temperature and Density of Classical Polydisperse Fluids, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Trusler, J.P., Extremely Accurate Measurement of the Speed of Sound in Gases, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 25, 1985.

Albright, P.C., A Crossover Description for the Thermodynamic Properties of Fluids in the Critical Region, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 27, 1985.

Gallagher, J.S, An Equation of State for Isobutane-Isopentane Mixtures with Corrections for Impurities, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 27, 1985.

Edwards, T.J., Heat Capacity of Carbon Dioxide Near the Critical Point, Ninth Symposium on Thermophysical Properties, University of Colorado, Boulder, CO, June 27, 1985.

MacDonald, R.A., A "Gel" Model for Coal, Gordon Conference on "Fuel Science," New Hampton School, NH, July 1, 1985.

Moldover, M.R., Critical Phenomena in a Low-Gravity Environment, Division of Policy Research and Analysis, National Science Foundation, Washington, DC, July 10, 1985.

Pegg, I.L., Tricritical and Critical-End-Point Phenomena in Fluid Mixtures; Phase behavior and Interfacial Tensions, Thermophysics Division Colloquium, NBS/CCE, Gaithersburg, MD, July 25, 1985.

Albright, P.C., A Crossover Theory for Fluids, Gordon Conference on Physics and Chemistry of Liquids, Holderness School, Plymouth, NH, Aug. 19, 1985.

Moldover, M.R., Optical Studies of Wetting Layers, Gordon Conference on Physics and Chemistry of Liquids, Holderness School, Plymouth, NH, Aug. 22, 1985.

Moldover, M.R., Critical Phenomena in a Low-Gravity Environment, Gordon Conference on Gravitational Effects in Materials Processing and Living Systems, Colby-Sawyer College, NH, Aug. 23, 1985.

Guzman, F., Foam Stability and the Wetting-Nonwetting Phase Transition, Thermophysics Division Colloquium, NBS/CCE, Gaithersburg, MD, Sept. 6, 1985.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

P.C. Albright

NBS Child Care Center (Board of Directors)

A. Cezairliyan

International Organizing Committee of the European Thermophysical Properties Conference (Member)

Thermophysical Properties Committee of the American Society of Mechanical Engineers (Member)

International Thermophysics Congress (Chairman)

International Commission on Standardization of Thermophysical Measurement Techniques (Member)

Thermophysical Properties Subcommittee of ASTM (Member)

E. Clark

ASTM Committee E44 on Solar Energy (Member)

ASTM Committee G3 on Durability of Nonmetallic Materials (Member)

L. Haar

International Association for Properties of Steam, Working Group I, Equilibrium Properties (Member)

International Union of Pure and Applied Chemistry, Subcommittee on Thermodynamic Properties of Ammonia (Member)

NBS Library Committee (Member)

NBS Editorial Review Board (Member)

J. Hubbard

NBS Colloquia Committee (Member)

J. Kincaid

NBS Storeroom Committee for ADP (Chairman)

G. Morrison

Subcommittee on Estimation of Thermal Properties, Design Institute for Physical Property Data of the AIChE (Member)

R.D. Mountain

NBS Library Subject Specialist Committee (Member)
NBS User Committee for Scientific Computing (Chairman)

J.M.H. Levelt Sengers

International Association for Properties of Steam, Working Group A, Thermophysical Properties of Light and Heavy Water and of Aqueous Systems (Chairman)

ASME Research Committee on the Properties of Steam (Member)

J.V. Sengers

ASME Research Committee K-7 on Thermophysical Properties (Member)

ASME Research Committee on the Properties of Steam (Member)

International Association for Properties of Steam, Working Group A, Thermophysical Properties of Light and Heavy Water and of Aqueous Systems (Member)

IUPAC Commission I.2 on the Transport Properties of Fluids (Corresponding Member)

EDITORSHIPS

A. Cezairliyan

Book, Compendium on Thermophysical Properties Measurement Methods, Plenum (Editor)

Book, Specific Heat of Solids, McGraw-Hill (Editor)

International Journal of Thermophysics (Editor-in-Chief)

Journal of High Temperature Science (Member, Editorial Board)

Journal of High Temperature-High Pressures (Member, Editorial Board)

A.P. Miiller

Book, Specific Heat of Solids, McGraw-Hill (Coeditor)

J.V. Sengers

Physica A (Member, Editorial Board)

International Journal of Thermophysics (Member, Editorial Board)

9. PROFESSIONAL INTERACTIONS

INDUSTRY

P. Albright

Collaboration with J.F. Nicoll, Pangaro Inc., in the general area of field-theoretical calculations in critical phenomena.

J.M.H. Levelt Sengers

Interactions with R. Basu, Allied Chemicals, on properties of near-critical solvents.

ACADEME, NATIONAL LABORATORIES AND GOVERNMENT

P. Albright

Collaboration with J.V. Sengers and J. Chen, University of Maryland, on several aspects of the crossover behavior of fluid systems.

A. Cezairliyan

Cooperative research with the Italian Metrology Institute, in the area of melting point measurements.

Cooperative research with the Air Force Materials Laboratory, in relation to thermal properties of aerospace materials.

Cooperation on thermal properties measurements with K. Maglic of Boris Kidric Institute, Yugoslavia, in connection with U.S.-Yugoslavia scientific cooperation.

Cooperative research with international laboratories, in connection with the CODATA Program on reference materials for thermophysical properties.

Cooperative research with the IUPAC Commission, on high temperatures in connection with secondary temperature standards.

Consultant, CINDAS/Purdue University.

L. Haar

Collaboration with G. Ernst, University of Karlsruhe, Germany, on the ideal gas-calorimetric temperature scale.

Collaboration with W. Wagner, University of Bochum, Germany, on thermodynamic properties of fluids.

J.B. Hubbard

Collaboration with P.J. Stiles, Macquarie University, Australia, on hydrodynamics of magnetic and dielectric colloidal suspensions.

Collaboration with P.G. Wolynes, University of Illinois, on theories of solvated ion dynamics.

Collaboration with J. Mercer, NBS, F. Martinez, University of Puerto Rico, and R. Dorfman, University of Maryland, on inhomogeneous chemical reaction kinetics.

Collaboration with J. Rasaiah and S.H. Lee, University of Maine, on diffusion-controlled reaction kinetics - theory and computer simulations.

J.M. Kincaid

Cooperative research with J. Erpenbeck at Los Alamos Scientific Laboratory, on computer simulation of transport processes in fluids.

Cooperative research with G. Stell of SUNY (Stony Brook), E.G.D. Cohen and M. Lopez de Haro of Rockefeller University, on kinetic theory.

Collaboration with J.K. Percus, Courant Institute, New York University, on theories of interfaces.

R.A. MacDonald

Cooperative research with R.C. Shukla, Brock University, St. Catherines, Canada, on thermophysical properties of bcc metals.

Collaboration with J.E. Callanan and S.A. Sullivan, NBS/CCE, Boulder, on heat capacity of coal.

M.R. Moldover

Collaboration with A. Voronel, University of Tel Aviv, Israel, on measurements of properties of alkali metal alloys (U.S.-Israel Binational Science Foundation Agreement).

Collaboration with J. Mehl, University of Delaware, on acoustic measurements in gases.

Collaboration with R. Gammon, University of Maryland, on measurements of transport properties near critical points.

G. Morrison

Collaboration with D. Didion, M. McLinden, and P. Domanski, Building Equipment Division, NBS/CBT, on Refrigerant Mixture Properties and Modeling.

R.D. Mountain

Collaboration with P.K. Basu of the University of the District of Columbia, on liquid state studies.

Collaboration with M. Klein, National Research Council of Canada, on gas hydrate studies.

Collaboration with R. Mazo, University of Oregon, on triplet-correlations in lipid membranes.

J.W. Schmidt

Collaboration with W.B. Daniels, University of Delaware, and M. Nielsen, Denmark, on neutron scattering from solid deuterium.

Collaboration with R.T. Jacobsen, University of Idaho, R.D. McCarty, NBS/CCE, J.V. Sengers, University of Maryland, and W. Wakeham, Imperial College, UK, on IUPAC book on ethylene.

Interactions with De Swaan Arons at Technical University of Delft, The Netherlands, preparatory to applying for NATO grant for collaboration on supercritical fluid mixtures.

Collaboration with K.S. Pitzer, University of California, Berkeley, on near-critical aqueous electrolyte solutions.

Interactions with R.W. Wood, University of Delaware and with W. Marshall and J. Simonson at Oak Ridge National Laboratory, on high-temperature, high pressure aqueous solutions.

Interactions and planned collaboration with M. McHugh, Department of Chemical Engineering, Johns Hopkins University, on polymeric solutions at high pressures.

Lab visit to R. Kobayashi, Department of Chemical Engineering, Rice University, March 1985.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

Ninth Symposium on Thermophysical Properties, held June 1985 in Boulder, CO. A. Cezairliyan and J.V. Sengers Symposium Board Members.

Conference on Electrolyte Solutions in Science and Engineering, held June 10-12, 1985, at NBS, Gaithersburg, MD. Organized by J. Rasaiah and J. Hubbard.

Gordon Conference on the Physics and Chemistry of Liquids, held Aug. 19-23, 1985, in Holderness School, Plymouth, NH. Chaired by J.M.H. Levelt Sengers.

Working Group A, International Association for Properties of Steam, meeting held Sept. 15-20, 1985, at NBS, Gaithersburg, MD. Chaired by J.M.H. Levelt Sengers.

European Conference on Thermophysical Properties, to be held in Sept. 1986 in Rome, Italy. A. Cezairliyan, international organizing committee member.

WORKSHOPS

Hosted workshop on Supercritical Solvents, held Oct. 17-18, 1985, at NBS, Gaithersburg, MD. Organized by J.M.H. Levelt Sengers.

SEMINARS

R. Lipowsky, Cornell University, Baker Laboratory, Ithaca, NY: Critical Effects of Wetting, Oct. 1, 1984.

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A. Robledo, Division De Estudios De Posgrado, Universidad Nacional Autonoma De Mexico, National University of Mexico, Mexico City, Mexico: Relationships Between Wetting Behavior and the Stability of Transient Foams and Emulsions, Sept. 20, 1985.

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TECHNICAL ACTIVITIES
OF THE
CHEMICAL PROCESS METROLOGY DIVISION (775)

J.J. Ulbrecht, Chief

1. INTRODUCTION

The end of FY85 marked the first year of the Division's reorganized operation. Since October 1984, the four constituent groups of the Division have been Fluid Flow, Multiphase Reacting Flows, High Temperature Reacting Flows, and Process Sensing. The motivation for the restructuring of the Division was thoroughly discussed in the 1984 Annual Report and need not be repeated. The reprogramming of the Division, which followed, was the chief characteristic of this past year.

When reviewing the performance of this past year, we need to examine how new programs were phased-in and old programs strengthened, while building on the existing skills and expertise of the four groups. We need to assess the means and ways by which these changes were enacted and implemented.

Among the traditional tasks the Division is entrusted with is instrument testing and calibration. A large number of industrial companies and government agencies (both military and civilian) rely on this service. The Division provides the custody, maintenance, and development of national reference standards for fluid flow, air speed, volume, liquid density, and humidity; and thus provides industry with traceability of their process instrumentation to primary national standards. In view of the importance of this task, the Division has undertaken, over a period of several years, substantial upgrading and automation (as appropriate) of all its calibration facilities which will result in substantial reduction of measurement uncertainties.

A number of ongoing research projects were identified as being of fundamental importance to the pursuit of the Division's mission and these were earmarked for further support. While a list of these is given in the main body of this report, several should be specifically noted. The research on droplet break-up and on bubble shedding is progressing satisfactorily and intermediate results were presented at national meetings. The slurry flow loop, which has been perfected, is now being readied for testing of slurry meters. The consortium research project, on the stability of vortex flow downstream from a strut, has generated a wealth of new data which aid in understanding the performance of vortex shedding flowmeters. The application of the RF meter, to the measurement of solids concentration in a paper pulp slurry, has reached the point of construction of a sturdy full scale model to be tested in a paper mill. The project concerned with the determination of discharge coefficients of orifice plates is nearing completion, and the indications are that its results will be a landmark in the history of flow metrology.

The high speed laser tomographic technique has been substantially improved by being extended to six angular positions so that nonsymmetric flow fields can now be studied. Important discoveries were made in the study of spray combustion: significant coalescence takes place downstream in the jet even under hot conditions. New data were obtained for the oxidation rate in diffusion flames which allow for further quantification of the kinetics of soot formation. Important advances were achieved by applying the new optical probe to the investigation of solids mixing in gas fluidized beds. These new data will serve to optimize catalyst regeneration rates.

In the field of process sensing, solid state sensors are emerging as contenders for a leading position. They are robust, stable, and reliable. In following this trend, the search continued for the basic understanding of how to apply iridium oxide to pH sensing. Humidity measurement in air and other common gases has remained one of our major research thrusts. The work on polymer membrane sensors has resulted in a patent being awarded to Dr. P. Huang.

Even though the progress in the above mentioned projects is indicative of the Division's effort, it does not give the full picture of the progressive reprogramming of the research thrust.

The FY85 year marks our entry into the arena of biochemical engineering. Next year we will report first results in developing the technique based on laser induced fluorescence to the measurement of intracellular kinetics. This noninvasive optical probe can provide a comprehensive signature of metabolic intermediates which is uniquely indicative of the complex kinetics of biochemical reactions.

In cooperation with the University of Paris we have started work on a new electrochemical method, which will make it possible to measure diffusion coefficients of oxygen in rheologically complex media (such as fermentation broths or gels) and, in parallel, determine critical shear rates in fermenters.

A new project has been initiated in cooperation with the University of Maryland, building on exploratory work recently completed here by a visiting Texas A & M faculty member, on the use of ultrasound probes to measure biomass concentration and cell viability.

A natural outgrowth from the soot formation project is a new project concerned with the formation of noncarbonaceous particles in high temperature reactions. This is an exciting field, impacting on the microelectronics fabrication industry and the ceramics industry.

Over the years, we have developed a capability to measure the response to radio frequency microwaves in heterogeneous materials. A new venture in this field is the use of guided microwaves to measure the dielectric constants in different coordinate directions and thus, in turn, the flow anisotropy. Application of this principle is expected in the field of on-line control of flow oriented materials (such as liquid crystals or composites) and in rheological testing of nontransparent materials.

Our new surface analytical facility has finally come on stream. This is a very powerful tool for studying surface structures and the nature of surface bonding forces. We expect it to provide an invaluable service in the investigation of the physical and chemical transformations taking place on the interface of solid state sensors, and in the study of gas-solid chemical reactions.

The progressive reprogramming of the Division's research thrusts would not have been possible without active participation of Group Leaders and senior research staff. It is mainly due to their imagination and creativity that so much of the existing expertise could have been reoriented towards the needs of the chemical and processing industries, and that new applications of ongoing projects were identified.

To catalyze the process of reprogramming, the Division entertained a number of seminar speakers who came to talk about new chemical engineering ventures. We had visiting faculty working with us over the summer period who helped in getting us started in new areas and who taught us their special skills. Two minicourses were organized during the past year: one on the design of novel chemical reactors (with particular emphasis on chemical vapor deposition) and the other on biochemical reactors. We have formalized three agreements on expanded research cooperation, one with Lehigh University in the area of biochemical engineering, another with the University of Maryland on sensors, and a third with the University of Tennessee on process measurement and control. These three agreements will provide for the exchange of staff and for joint supervision of graduate students working on projects of mutual interest.

An important tool in the reprogramming process was the sponsorship of three workshops, attended by representatives from industry and academia. One workshop dealt with process measurement of rheological parameters, and our new project in flow birefringence in opaque materials is in direct response to the recommendations of this workshop.

Another workshop, jointly sponsored by the Center for Biotechnology at Lehigh University, dealt with process measurements for biochemical reactors. One of the conclusions of this workshop was that, in the absence of inexpensive NMR process instrumentation, spectroscopic measurement interfaced with advanced fiber optic probes is the most plausible process instrumentation to monitor reaction kinetics along complex pathways. We have incorporated these recommendations into our infrared and laser induced fluorescence projects.

A third workshop, also cosponsored by Lehigh University, was concerned with the scale translation and design of bioreactors. The participants emphasized the need for fundamental design data and standardized measurement techniques. We anticipate that the bulk of these recommendations will be included in our long range plan. For the time being, we have started the diffusion coefficient project.

The latter two workshops produced a fairly sharp picture of the current needs of the biotechnology industry. We utilized the results of these workshops when writing the FY87 Budget Initiative on "Bioprocess Engineering."

We have continued cultivating the widest possible contacts with the chemical and processing industries, either through trade organizations or through consortia of companies, to assure the societal relevance of our research work. A new industrial consortium was recently formed in support of a research project on flow conditioning. Discussions with several industrial companies to determine their interest in the measurement of critical shear rates, and in the measurement of flow birefringence by microwave frequencies, are in progress.

2. GOAL

Within the framework of the Center for Chemical Engineering, the Chemical Process Metrology Division's main concern is the science of measurement in homogeneous and heterogeneous flow systems with and without chemical reactions.

The goal of the Chemical Process Metrology Division is to provide the chemical and related industries and other government agencies with the measurement techniques, fundamental data, and the underlying scientific principles pertinent to homogeneous and heterogeneous flows, with and without chemical/biochemical reactions, at ambient and elevated temperatures.

The key element in the pursuit of this goal is the integration of transport processes taking place in the spatial and temporal environments of a sensor with the physical, chemical, and biological transformations taking place at the interface of the sensing element.

It is further recognized that process measurement is the key component of any process control loop, the proper function of which is essential to the maintaining of the highest quality of manufactured goods and, in turn, of the competitive edge of the U.S. industry on domestic as well as foreign markets.

Parallel with its research work, the Division maintains state-of-the-art calibration services for flow, volume, density, humidity, and airspeed; providing industry and other government agencies with traceability of their instrumentation to national standards and thus assuring equity in domestic and international trade.

3. GROUP FUNCTIONS

o Fluid Flow Group - G.E. Mattingly, Group Leader

The mission of the Fluid Flow Group is to study the fundamentals of fluid flow with the aim of advancing the state-of-the-art in flow metrology and of applying these principles toward improving and expanding the flow measurement capabilities for gases, liquids, and multiphase systems.

Research areas in the Group focus on fluid mechanical studies of fluid flow phenomena in closed conduits as well as in less confined configurations --such as exemplified by fluid mixing geometries pertinent to the chemical process industries. Specific research programs have focused on flowmeter installation effects, i.e., the influence of nonideal piping configurations on downstream meters, on the generic performance of specific flowmetering techniques such as vortex shedding, and on fluid handling and measurements in unusual conditions such as in zero gravity environments or in complex flows such as solid-liquid slurries.

The Fluid Flow Group has maintained responsibility for the fluid flowrate and airspeed calibration services requested of the Center in FY85. Additionally, the Group has maintained the central responsibility for the calibration-upgrade activities being carried out for all of the calibration services offered within the Center. These upgrade activities will describe, quantify, and in the coming year report the levels of uncertainty for our measurement procedures that constitute our calibration services.

Significant among the Group's activities in the past year is the topic of flow measurement assurance and strengthening the "links" in appropriate traceability chains. A number of critical "in-situ" calibrations were carried out to prove a number of diverse flowmeter installations for U.S. industries, especially the nuclear industry. Also, a number of projects have been initiated to conduct interlaboratory or round-robin flowmeter testing programs, to assess systematic errors that may exist between or among flow measurement laboratories.

o Multiphase Reacting Flows Group - G. Kulin, Acting Group Leader

The mission of the Multiphase Reacting Flows Group is to conduct research on multiphase flows at ambient and near-ambient temperatures with and without chemical reactions. The ultimate purpose of this activity is to (1) provide fundamental data, (2) develop improved measurement techniques, including on-line rheometric methods, and (3) develop physical and mathematical models for improved understanding and control of physical and chemical processes in low temperature reactors, particularly biochemical, slurry, and polymerization reactors. Examples of current research include investigations of (1) droplet breakup in mixer-blade flowfields, (2) bubble generation and behavior near mixer blades, and (3) initiation of a study of liquid fluidized beds, which represents an extension and redirection of Group interest in hydraulic transport of solids. Further redirection of the program to accommodate new aspects of the Group's mission is evidenced in recently started projects on electrochemical methods of shear stress and diffusion measurement, and on microwave birefringence techniques for determining flow-induced anisotropy in polymers.

o High Temperature Reacting Flows Group - H.G. Semerjian, Group Leader

The High Temperature Reacting Flows Group conducts fundamental research on chemically reacting multiphase flow systems, especially those involving dispersed particles either formed during the process (e.g., soot formation during combustion), or entrained into the flow stream (e.g., fixed or fluidized beds, sprays, etc.), and on development of advanced measurement techniques applicable to chemical reactors. Primary focus of the Group's activities has been the development of nonintrusive measurement techniques applicable to high temperature (and pressure) reactors. Recent efforts have included studies on laser tomography for temperature and composition measurements, laser scattering and extinction for particle characterization in sooting flames or sprays, laser induced fluorescence for temperature measurements in flames, emission spectroscopy for temperature measurements in industrial reactors, and fiber optic probing techniques in fluidized beds. Some of these techniques are being extended into new areas of research. For example, the laser scattering and extinction techniques will be applied to studies of particle formation processes relevant to CVD systems, as well as to ceramics and powder metallurgy; the laser induced fluorescence techniques are being applied to biochemical systems, where they are expected to provide a powerful tool for measurement of substrate and product concentrations, as well as the metabolic activity level and intracellular kinetics. New laboratory facilities are also being established (e.g. the new plug flow reactor) which will enable study of transport and reaction rates in multiphase flow systems, relevant to pyrolysis and oxidation of heavy fuels, slurries, process biproducts, and hazardous wastes.

o Process Sensing Group - S. Hasegawa, Acting Group Leader
J.R. Whetstone, Group Leader

The Process Sensing Group performs research directed toward the development of new sensing and measurement techniques. We have the capability to make a broad spectrum of sensing materials in the form of thin films, using sputtering. Surface adsorption/desorption phenomena may be characterized using the new surface analytical facility which was commissioned in June of 1985. Initial efforts here have dealt with the thermal desorption and surface bonding characteristics of tin oxide, which is a semiconducting oxide having demonstrated affinities for absorption of water vapor and other gaseous species. Additionally, iridium oxide films which hold promise as solid state pH sensors have been made. Preliminary studies of the relationship between fabrication parameters and structure of the films as well as electrical properties have been made. This work will be followed by surface characterization to determine the mechanism of the film's pH response. The sputtering facility has been used to develop thin film thermocouples on metals. An extension of this work includes the study of application of thin film thermocouples to ceramic and polymeric materials.

The Process Sensing Group bears the responsibility for NBS calibration services for volumetric, density and humidity measurement devices. Preparations have been made to recompare the response of the two-pressure humidity generator to the gravimetric hygrometer, perform surveillance checks on the volumetric working standards using gravimetric techniques, and to develop a set of fluids to be disseminated as standard density reference materials.

4. SELECTED PROJECT SUMMARIES

CALIBRATION

Calibration Services

G.E. Mattingly, S. Hasegawa

In the past year the CCE calibration services have satisfied industry and government requests for a number of metrological tasks. Additionally, the facilities for performing these services are being upgraded so that the levels of measurement uncertainty are being evaluated. Where pertinent, improvements are being made; where appropriate, automation of procedures is being implemented. In the specific calibration areas, activities are summarized as follows:

Service	Number of Items Calibrated
Flowrate	33 (26 for industry)
Volumetric Containers	53 (51 for industry)
Aerodynamic Devices	84 (42 for industry)
Reference Standard Hydrometers	60 (60 for industry)
Humidity	25 (21 for industry)

Besides these services, an increasing number of "in-situ" calibrations were performed by NBS personnel. In this way, improved measurement assurance was provided to strengthen the traceability links between actual, installed instrumentation and the national standards for these measurements.

In the area of humidity calibrations, a microprocessor has been interfaced with the humidity calibration facility to automate the calibration of hydrometers. The volumetric transfer standards were verified via gravimetric calibrations.

FLUID FLOW GROUP

An Investigation of Organized Motions in Coflowing Streams

R.W. Davis

A joint computational/experimental investigation of the entrainment process in the mixing of a round jet with a coflowing stream has been carried out. The overall objectives of this work were to identify and characterize coherent motions in the mixing region, investigate the dynamic role these motions play in the entrainment process, and determine the extent to which entrainment is affected by such factors as initial conditions and forcing. The computational portion of this investigation produced numerical models for forced spatially-developing axisymmetric and two-dimensional mixing layers. It was shown that the vortex merging behavior in both types of mixing layers is determined by the subharmonic content of the forcing function. It was found experimentally that linear parallel flow stability theory agrees qualitatively with measurements, but does not produce accurate quantitative predictions of spatial growth rates. It was also found that the previously used scaling laws describing the character of the initial jet instability need to be changed. Replacement scaling laws have been advanced and verified and are based upon the average of the jet and local minimum speeds. With these new scaling laws, improved descriptions can now be made of the initial entrainment and mixing processes.

A Vortex-Induced, Liquid Handling and Accountability Procedure at Zero Gravity

T.T. Yeh, R.W. Davis

A two-stage process for handling two-phase, i.e., gas-liquid fluid systems in cylindrical tanks at zero gravity has been modeled using analytical and computational techniques. The initial "spin-up" stage is established by tangential fluid injection. A simplified model of this stage has been developed using several phase interactions such as fluid drag and virtual mass effects. The results of the spin-up stage predict the gas-liquid separation characteristics as liquid centrifuges to the outer wall of the circular tank, leaving the gas to occupy the center core region.

The second stage "pump-out" from the tank is modeled using an NBS-developed code which computes forced liquid withdrawal from the cylindrical tank. The results give complete velocity and pressure conditions for the drawdown process.

The two stages form a composite description for a range of parameters that can be tested and evaluated for their influence on liquid handling and accountability at zero gravity. Experimental verification is needed for a number of the simplifying assumptions and the accuracy of the predictions of the models.

Flow Installation-Effects Research

G.E. Mattingly, T.T. Yeh

An NBS-DOE funded research program has been initiated to produce effective flowmeter installation specifications that are critically needed for improved fluid measurement standards. Because the planned results of this program impact the entire fluid metering community, an industry-government consortium is being formed to accelerate progress and enable industry - both meter manufacturers and users alike, to participate, to use the results, and to guide subsequent phases of the research. The strategy adopted for this program contrasts markedly with that used in the past. Conventionally, it has been the practice to conduct very considerable numbers of specific meter calibrations to determine the minimal distances (between meter and piping configuration) for which uncertainty levels on meter factors are to be increased by specified amounts. Through this conventional approach, little was learned about the salient features of the pipeflow profiles involved. The currently adopted strategy focuses on these profiles - specifically - without any flowmeter, measures these profiles using Laser Doppler Velocimetry (LDV), and characterizes them and their changes with distance from the piping configuration. With these results a number of organized, informed calibration tests can be carried out by meter manufacturers and others so that specific results, i.e., discharge coefficients, meter factors, etc. are thereby related to pipeflow characteristics. In this way, meters can be installed in any locations where their performance is satisfactorily stable and meter factors or discharge coefficients predicted for the installation. It is expected that this strategy will produce installation specifications for metering standards which will enable satisfactory flow measurements to be made in less-than-ideal circumstances. Subsequent phases of this research have been suggested by industry participants to focus on the effectiveness of flow conditioners for achieving improved meter performance in nonideal meter installations.

Vortex Shedding Flowmeter Research

G.E. Mattingly, T.T. Yeh

An industry-government consortium has been formed to conduct a program of research on the stability of vortex shedding in a generic vortex shedding flowmeter geometry. Current consortium participation consists of flowmeter manufacturers and users from the U.S. and abroad. This two-year program uses the Laser Doppler Velocimetry (LDV) system to measure vortex characteristics in the generic meter geometry through a range of closely controlled conditions. Research results are provided to the consortium membership via regularly scheduled meetings and reports. Ultimately, the results of this program will be published in the open literature. Consortium members who are meter users (or potential users) will benefit from having unique data describing vortex shedding flowmeter performance. These results and those expected from successive phases of this research are expected to produce improved performance from vortex shedding flowmeters.

Orifice Discharge Coefficient Database Development

G.P. Baumgarten, W.G. Cleveland, J.R. Whetstone, S. Woo

A fully documented database is being developed for flange tapped orifice meters. The currently used database was developed during the 1930's over a relatively small range of Reynolds numbers. NBS is nearing completion of two projects which cover the intermediate Reynolds number range (5,000 to 2,500,000) and the high Reynolds number range (50,000 to 14,000,000). The intermediate Reynolds number project is being done in the NBS-Gaithersburg laboratories and the high Reynolds number work is being done in collaboration with the Natural Gas Pipe Line Company of America (NGPLA) at their Joliet, Illinois, test site. NBS has developed the measurement systems used in the NGPLA tests and is reducing the data as it is acquired. Both projects are nearing completion with the final reports expected in 1986.

During 1985 it became clear that the effects of rust on the surface of the meter tubes caused considerable irreproducibility in the databases collected through December 1984. Extensive investigation for sources of this effect were made in the measurement systems, and in effects of surface roughness caused by rust on the meter tube surfaces. The measurement systems were found to be performing properly. After a considerable amount of testing, it was shown that the effects of relatively small, rapidly formed amounts of rust were the cause of irreproducibility in the data. Various corrosion inhibition methods were investigated without success. Finally, the solution to the problem was found in the application of a 25 μm plating of electroless nickel to the interior of a single meter tube. Test results of that meter tube showed excellent reproducibility. Corrosion on the surface of the meter tube was eliminated. The remainder of the meter tubes were electroless nickel plated and the entire database has been reproduced with uniformly good results. Completion of data collection is expected in December of 1985. A second round of tests at NGPLA were also completed.

The results of these projects combined with similar data in the low Reynolds number range are expected to form the basis for a new orifice meter flow measurement standard to be promulgated by the American Petroleum Institute.

Drop Extension and Breakup in Mixer Blade Flow Fields

R.C. Calabrese, N. Bryner

A liquid-liquid drop dispersion flow loop facility has been constructed, in collaboration with the University of Maryland, to study the deformation and breakup of drops in the vicinity of sharp-edged bodies which simulate real mixing elements. The facility uses laser velocimetry, high speed photography, and the hydrogen-bubble technique to characterize flow fields and drop behavior. Initial laser-velocimeter results for the unobstructed test section were presented at Mixing Conference X, Henniker, New Hampshire, in August, 1985. These data suggested that the settling chamber and converging section are removing large scale turbulence and providing desirable velocity profiles, but more data must be collected to better understand the flow field before the mixer element is installed. The early data also indicate that the hydrogen bubble technique must be used to visualize the flow around the blade before taking further laser velocimetry measurements. The flow visualization technique will permit crude studies of velocity gradients and shear fields. The preliminary studies will dictate which areas around the blade must be studied further and, after complete characterization of the flow, drops will be added to allow study of the deformation and breakup process. A mechanistic model for drop stability is being developed concurrently.

On-Line Consistency Measurement

A.K. Gaigalas, J.R. Whetstone

The objective of this project is the development of an accurate, non-intrusive measurement technique for on-line global sensing of consistency (solid-phase fraction) in paper pulp flows. The technique utilizes interference effects on radio frequency waveguides. The waveguide is a part of the piping system carrying the slurry. Recent efforts were directed toward scaling up the technique to a six-inch diameter pipe size from the two-inch diameter prototype on which experiments had been completed earlier. A six-inch diameter prototype was constructed and has been successfully tested in the pulp loop at the Institute for Paper Chemistry in Appleton, Wisconsin. Currently, a version of this meter, suitable for use in an actual paper mill environment, is under development.

Formation of Bubbles in Shear Flows from Orifices

A.K. Ghosh, J.J. Ulbrecht

The process of bubble formation from submerged orifices in a moving continuous phase of rheologically complex liquids is being investigated. Both experimental and numerical techniques are used to determine the bubble growth rate during the formation of gas bubbles and the final bubble size. Unlike the earlier models published in the literature, this new model does not assume a spherical shape of the bubble, nor does it introduce an artificial condition of detachment. Further, it allows for the inclusion of a drag force exercised either by a Newtonian or non-Newtonian liquid flowing past the bubble. The influence of various parameters on the bubble size is also being studied by varying the gas flow rate, liquid phase velocity, orifice diameter, and the liquid height. A high-speed photographic technique is used to determine the actual bubble profile and the detachment criteria. The photographic images are digitized using an image analyzer.

Both the experimental and numerical results, obtained so far, indicate that the superimposed liquid drag reduces significantly the growth period and thus the final bubble size. The agreement between the experimental and numerical results is very encouraging. The project provides a basis for the modeling of gas-liquid contactors, such as stirred-tank reactors, biochemical reactors, bubble columns, and distillation trays.

Formation of Bubbles in Shear Flow from a Gas-Filled Cavity

K. Yuk, J.J. Ulbrecht

The mechanism of gas dispersion in liquid in a stirred tank is simulated by a rotating flow past a stationary blade. The gas cavity behind the stationary blade is formed by feeding air directly into the downstream side of the blade, and is found to be similar to those observed behind rotating stirrers. The local size distribution of the gas bubbles redispersed from the tip of the cavity will be determined with a photoelectric capillary probe. The effect of Newtonian and non-Newtonian liquid properties and flow parameters on the bubble size will also be investigated. The force acting on the blade is measured by a strain gage mounted on the blade arm, and can be used to determine the power requirement of the stirrers.

Solid-Liquid Flow Loop

G. Kulin, K.E.B. Lofquist

The solid-liquid flow loop now in operation has two important features: capability for continuous operation with solids by-passed around the pump, and essentially constant flowrate of solids for a given hopper opening, regardless of changes in water flowrate or settling-out of solids within the loop. Several minor modifications to the loop were made to enhance its performance, including an additional air-cushion surge tank, a modified elbow upstream of the test section, and improved pressure-drop measurement capability. Experiments were completed in which light was transmitted chordally across the two-inch transparent pipe at several locations, detected, and analyzed with a signal processor as a check on uniformity of flow conditions along the test section. These measurements ensure that observed concentration fluctuations are not caused by the lock rotation or upstream elbow. A theoretical-empirical model for velocity and concentration distribution in the flow was developed. Plans are being made to develop the loop as a slurry metrology test facility.

Solid Phase Distribution Measurement Using X-Ray Tomography

J.R. Whetstone, D.S. Loebbaka

The simultaneous measurement of the solid and liquid phase concentration and distribution, in solid-liquid systems, may be accomplished in a nonintrusive manner using the tomographic reconstruction method. Considerable effort has been devoted to an alternative technique, based on Compton scattering of X rays rather than the generally used transmission method. Such a technique reduces the mechanical complexity of the device considerably. Feasibility experiments resulted in the decision to continue with the transmission technique. The first prototype was used to measure chordal average solid-phase concentrations, along seven approximately horizontal and equally spaced chords, in a horizontal plastic pipe two inches in diameter. Measurements were successfully completed on a flow of 0.55 mm sand particles (in water), at concentrations ranging from near-deposit conditions at the bottom of the pipe to essentially zero near the top, with estimated accuracies of $\pm$ 5 percent.

Measurement of Shear Rate Near a Stirring Blade

B. Robertson

Apparatus for this measurement is being assembled. The shear rate is measured electrochemically in a salt solution flowing by the blade. A microelectrode is inserted flush with the surface of the stirring blade where the shear rate is to be measured. If a large voltage is applied to the electrode all of the ions at the surface of the electrode will react so that their concentration will vanish there. These ions are replaced by ions diffusing from the bulk of the fluid. The electric current, which is proportional to the rate of reaction at the electrode, is limited by this diffusion. Flow of the fluid tangential to the wall brings the ions more rapidly to the electrode, and so increases the current in a predictable way.

A rotating disk apparatus, which uses the same electronics, has been set up for measuring the Schmidt number. The technique has been developed recently by C. Deslouis and B. Tribollet in Paris and transferred to us last summer. The speed of rotation of the disk is modulated sinusoidally, and the resulting sinusoidal variation in the limiting current is measured. Comparison with theory yields the Schmidt number directly, without having to know the concentration of the diffusing species or the active area of the working electrode on the rotating disk. This technique will also be used to measure the diffusivity of oxygen in aqueous solutions.

HIGH TEMPERATURE REACTING FLOWS GROUP

Particle Formation in High Temperature Processes

R.J. Santoro, J.J. Horvath, H.G. Semerjian

Nonintrusive laser diagnostics are being applied to investigate particle formation processes in hydrocarbon flames. Detailed measurements of the soot particle fields using laser light scattering techniques have been obtained for a series of laminar diffusion flames. Complementary temperature and velocity measurements have been made in order to examine the effects of variations in the temperature and particle residence time on the soot growth process. Independent variation of the temperature in the flames has been investigated through the addition of inert diluents to the fuel and air flows. The experiments have demonstrated the strong temperature sensitivity of the soot formation process. Studies involving a series of fuel species (ethene, ethane, and methane), as well as a range of fuel flow rates, have elucidated the mechanisms responsible for soot particle escape from these flames. The importance of radiative transfer in establishing conditions conducive to soot particle production has been identified. The results of detailed soot growth calculations based on these studies are being used to form the basis of a soot formation model. More recently, experiments have been extended to a wider range of fuels including acetylene, propene and butene to examine the effect of fuel structure on soot formation. In these experiments, the temperature has been kept constant to isolate fuel structure (as a variable) from other effects. A prevaporization system has recently been completed to allow studies of liquid fuels under similar conditions. These studies are intended to examine soot formation under conditions more directly related to practical systems.

Efforts to understand the growth of particles in flames have also led to developments in the area of the application of optical diagnostics to particle size measurement. Measurements made in this laboratory have shown that, under certain conditions, light scattering measurements made on soot particles can exhibit incompatibilities with Mie theory predictions. These incompatibilities arise when measurements utilizing different scattering properties are used to obtain particle size. Our present efforts have concentrated on particle size measurements utilizing the ratio of scattering at two angles, the scattering-to-extinction ratio, and the polarization ratio. Each of these techniques yields an independent measure of the particle size. Efforts to bring these observations into agreement have examined two possible effects: the occurence of low density agglomerates, exhibiting markedly lower refractive index, and the presence of randomly oriented spheroids. Both of these approaches provide qualitative agreement with the experimental observations. Additional work is required to provide a more quantitative comparison. Presently, consideration is also being given to multiwavelength scattering measurements to provide more information on the particle nature. Efforts are also underway to investigate formation of particles other than soot. Metal particle sprays, silicon particle formation, and ceramic particle production represent novel research areas for application of similar techniques. A cooperative program, with the NBS Institute for Material Science and Engineering and the NBS Office of Nondestructive Evaluation, is being initiated this year to study metal particle formation processes.

Particulate and Droplet Diagnostics in Spray Flames

C. Presser, H.G. Semerjian, R.J. Santoro

Dynamics of spray flames are being studied to investigate droplet vaporization, pyrolysis, combustion,and particulate formation processes, and to delineate the effect of chemical and physical properties of fuels on the above processes. The results of this study will provide an experimental data base, with well defined boundary conditions, for the development and validation of spray combustion models being developed by JPL, Sandia, and Los Alamos National Laboratories. The experiments are being carried out in a spray combustion facility, with a moveable-vane swirl burner, which simulates operating conditions found in practical combustion systems. A combination of nonintrusive probing techniques is being used to obtain comprehensive data on the spray combustion characteristics, including soot particle and droplet size, number density and volume fraction, gas composition, and velocity and temperature fields.

Current efforts are focused on laser scattering and laser Doppler velocimetry measurements, which are being used to determine the correlation between droplet size and velocity distributions, respectively, in both low temperature and burning sprays.

High Speed Laser Tomography for Measurement of Concentration and Temperature Distributions in Reacting Flows

S.R. Ray, H.G. Semerjian

The technique of high speed laser tomography is under development to allow rapid measurement of temperature and chemical species concentration distributions throughout a two-dimensional "slice" within time-varying chemically reacting flow fields. Work has progressed from time averaged measurements of steady phenomena, such as laminar diffusion flames and gaseous jets, to real time measurements in sodium-seeded flames. Using the experience gained, the temperature and OH concentration field were measured in a premixed methane flame within five milliseconds. This was achieved by sweeping an ultraviolet laser beam through the field every millisecond while tuning the laser frequency over an OH absorption line. The experiment used an axially symmetric flame, requiring only a single measurement angle.

Current work has focused on rapid measurements in nonsymmetric fields at repetition rates up to 10 kHz, using a six angle tomography approach. The new system has been used to measure the particle concentration field in rapidly fluctuating flames. As a parallel effort a number of alternative reconstruction techniques have been investigated, using computer simulations, to identify the approach ideally suited to this experiment. The maximum entropy method is found to be the most suitable, especially for reconstructing the field from a small number of projections (e.g. six angles).

Flame Temperature Measurements by Laser Excited Fluorescence

J.J. Horvath, H.G. Semerjian

A new nonintrusive temperature measurement technique, based on laser excited fluorescence, is being developed for measurements in high-temperature chemically reacting flows. In this method, an upper electronic state is populated from the ground state by means of laser excitation. The population in this excited level is collisionally redistributed, then radiatively decays, and the resultant fluorescence is detected as a function of energy level. The temperature is then obtained from the plot of fluorescence intensity vs. energy, which yields a straight line due to the presence of a local Boltzmann distribution throughout the higher energy levels. The fluorescence observed is antiStokes of the excitation pulse, hence this method is applicable to high luminosity flames and conditions of high background Stokes fluorescence. This method is applicable to both naturally occurring species such as OH, CH, and C_2 or atomic species seeded into the flame. Initial experiments have used gallium as the seeding species in premixed flames. A tunable dye laser, pumped by a nitrogen laser, is used to excite the $4P_{1/2}$-$5S_{1/2}$ transition of Ga at 403.3 nm and the resultant fluorescence from upper levels is observed. A wide variety of premixed flames were studied in order to determine the useful temperature range of this technique. Flames studied were $CH_4/Ar/O_2$, CH_4/Air, $C_2H_4/Ar/O_2$, and C_2H_4/Air. The temperature of these flames could be varied from approximately 1950 to 2500 K depending on flow conditions. Experimentally measured temperatures were found to be about 100-150 Kelvins below the adiabatic flame temperature calculated using the NASA computer program. Fluorescence signals were also obtained in an ethylene diffusion flame, but an unexpected broad band fluorescence was observed which yielded abnormally high temperatures. To correct for this broad band fluorescence interference, computerized data reduction schemes were developed. Experimental results in a CH_4 diffusion flame were presented at the Conference on Lasers and Electro-Optics in May 1985. Work continues on techniques which allow temperature measurements with a single 10 ns laser pulse in diffusion flames.

Optical Sensing in Bioreactors

H.G. Semerjian, J.J. Horvath

Recent advances in molecular biology have led industry and government agencies to recognize the economic potential for applying these advances in a diversity of industrial sectors, including the production of new drugs, food additives, and chemicals, and conversion of biomass, etc. However, implementation of these new technologies requires measurement capabilities which do not currently exist. Bioprocesses require a very closely controlled environment, normally realizable only in batch processes. This is mainly because of the complex kinetics of most bioreactions, separate periods of growth and product formation, biocatalyst degeneration, contaminant risks, and in mechanical difficulties of handling a rheologically complex material. Therefore, development of new on line measurement techniques is critical for future implementation of bioprocesses. Furthermore, nonintrusive measurement methods are desirable to avoid difficulties associated with sampling, contamination, long response time, etc.

Optical techniques, especially with the use of tunable lasers, provide the best potential for making nonintrusive, rapid, and selective measurements. Use of fiber optics can also enable the development of probes which are sterilizable, can provide measurements with good spatial resolution, and can be multiplexed to provide multipoint monitoring capability. Laser induced fluorescence, Raman scattering, and infrared absorption techniques will be utilized for measurement of key process variables such as cell mass activity, cell concentration, and concentration of substrates and products. As part of a recently initiated project, preliminary experiments have been carried out on fluorescence characteristics of amino acids, indicating good sensitivity. These experiments will be extended to dipeptides, polypeptides, and esters. Raman and resonance Raman scattering will also be utilized to provide more species selectivity. Fluorescence techniques are also expected to provide a powerful tool for cell activity and intracellular kinetics measurements.

Emission Spectroscopy for Control of Combustion/Gasification Systems

S.R. Charagundla, A. Macek, H.G. Semerjian

Currently available control techniques for gasifiers, black liquor recovery boilers, and other industrial boilers are usually based on stack gas analysis. In-situ monitoring techniques, explored in this project, offer fast response as well as specific advantages in developing control strategies for multi-burner systems and for staged combustion systems. The goal of this project is to develop in-situ (remote sensing) techniques, based on emission spectroscopy, for measuring temperatures and chemical species in high-temperature reactors.

One application of the ongoing emission spectroscopy work is in the black liquor recovery boiler. Investigations thus far have characterized the emission spectra (from actual black liquor recovery boilers) in the wavelength range of 300 nm to 800 nm, using a spectrometer equipped with an Optical Multichannel Analyzer (OMA). These data indicate that only the line emissions from sodium at 589 nm, mostly in self-absorption, and from potassium at 404.4 nm and 766.5 nm, are readily observed. The potassium line emissions have been investigated in the laboratory using premixed methane/air flames seeded with black liquor or potassium chloride solution mist. These laboratory investigations indicate that line emissions due to potassium at the two wavelengths (404.4 nm and 766.5 nm) can be used to calculate the gas temperature (assuming Boltzmann distribution) by the line intensity ratio technique. A 4-channel optical system has been developed, including a branched fiber-optic bundle, each branch being connected to a bandpass filter, photodetector, and amplifier. The system allows simultaneous measurements of intensities of the two potassium lines and the corresponding background (continuum) emissions. The four color system is interfaced with a personal computer equipped for simultaneous data acquisition on four channels. A prototype probe system is being assembled now for testing at a paper mill site. Successful application of this technique to black liquor recovery boilers would demonstrate its potential for use in other high temperature reactor systems.

In the other application of emission spectroscopy, an extensive set of pyrometric and spectroscopic (OMA) data have been obtained from the reactor of a coal-gasifier pilot plant (Mountain Fuel Resources, Inc.) by means of multichannel fiber optics. The data have led to significant conclusions regarding the conditions in the interior of the reactor. It has been shown that: (a) there are large and rapid temperature fluctuations inside the reactor even at nominally steady fuel and oxidant feed rates and (b) line and band emission spectra of alkali and earth alkali atoms and compounds (Li, Na, K, Ca, CaO, CaOH, CaCl) are consistently observable features, characteristic of the coal gasification process. It is concluded that temperature alone is not a reliable indicator for the purpose of gasifier process control and safety. However, simultaneous optical measurements of temperature and one or more characteristic spectral lines and/or bands are promising for the development of on-line process monitors.

Fundamental Studies of Black Liquor Combustion

A. Macek, N.D. Amin, S.R. Charagundla, H.G. Semerjian

Efficient operation of black liquor (BL) recovery boilers requires more fundamental information on combustion of BL droplets than is currently available. The problem of measurement of the pertinent combustion parameters is addressed by a joint project with the Institute of Paper Chemistry under DoE sponsorship. The NBS tasks of this joint project are directed toward studies of vaporization, pyrolysis, ignition, and combustion of dilute streams of BL droplets. Construction of a high-temperature dilute-phase plug flow reactor (DPFR), specifically designed for such studies, is almost completed. Prior to the operation of the completed DPFR, an auxiliary reactor utilizing parts of the DPFR has been constructed, tested, and used for BL droplet injection studies.

A positive-displacement technique, in which individual droplets are extruded from a hollow needle, was developed earlier in this project for on-demand generation of highly viscous droplets with diameters of the order of 1 mm. This technique has now been successfully modified to allow injection of BL droplets (60% solids) into high-temperature streams in the auxiliary reactor. High-speed photography has been used for (a) observation of the processes of BL droplet formation and detachment from the needle tip, (b) measurement of droplet diameters prior to detachment, (c) measurement of in-flight droplet diameters after detachment, and (d) velocities of droplets falling in a counterflowing hot gas stream. Droplet diameters in these studies were varied from 1.3 to 2.3 mm, gas temperatures from 1,000 to 1,350 K, and gas velocities (upward) from 1.7 to 4.2 m/s. These are the ranges of parameters projected for actual use in the DPFR.

The DPFR constructed in this project will also be used for investigation of pyrolysis and oxidation of other fuels (such as coal/water) as well as oxidative destruction (incineration) of hazardous wastes. In addition to high-speed photography, the diagnostic techniques planned for future studies, both with BL droplets and other fuels, include laser-based nonintrusive measurements and gas-chromatographic analysis of samples extracted from the reactor.

High-Temperature Oxidation of Chlorinated Hydrocarbons

H.G. Semerjian, R.J. Santoro, A. Macek

Control of products of incomplete combustion (PIC), generated during incineration of hazardous waste, requires an understanding of rates and mechanisms of oxidation and thermal decomposition of its principal constituents (mainly chlorinated hydrocarbons). The experiments to provide such an understanding should be performed under well-controlled operating conditions which simulate the critical operating parameters (i.e., residence times, temperature, and oxygen content of the gas stream) of full-scale incineration systems. A project to accomplish this goal has been initiated, under the sponsorship of EPA. So far, a literature review of the subject has been initiated, and plans have been made for experimental studies.

The key experimental apparatus for this study will be a high-temperature flow reactor, allowing reaction residence times of the order of seconds, with multiple access ports for both sampling and nonintrusive optical measurements at various reaction stages. This facility will be provided at NBS by adaptation of the dilute-phase plug flow reactor for droplet combustion studies, which is currently near completion. While later stages of this project may also include work with droplets of chlorinated hydrocarbons, it is anticipated that the initial studies will be done with gaseous reactants. The main modifications of the existing reactor, therefore, will include: (a) lines for metered injection of gaseous reactants at the upstream end of the reactor; (b) a movable probe for gas sampling; and (c) gas-chromatograpic analysis capability for small amounts of chlorinated species. The capability of attaining the desired temperatures (up to 1300 K), oxygen contents (0 to 21%), and gas residence times (1 s or more) -- as well as provisions for nonintrusive optical diagnostics -- are included in the basic design of the reactor. The flow capabilities of the reactor have already been demonstrated in the project on fundamentals of black liquor combustion.

Optical Measurements in Fluidized Bed Reactors

A. Macek, N.D. Amin

A high-temperature fluidized bed reactor is being maintained and instrumented for research toward development of advanced in-situ measurement techniques. The reactor has a square cross-section, 15x15 cm, and has a gas throughput capability of up to 150 cm/s at temperatures up to about 1150 K. The principal advance beyond the state-of-the-art probing of fluidized beds has been the development of an optical probe, allowing observations at one or more arbitrarily chosen locations in the interior of the bed. In the first application of the technique, reported previously, temperature measurements were obtained of burning particles inside the bed. The second application, currently in progress under DoE sponsorship, is a study of solids movement in fluidized-bed reactors. The study is based on the fact that a burning particle generates a distinct signal as it arrives at an optical probe location. The impetus for this study is the importance of the problem of mixing in fluidized beds, used in many chemical engineering processes.

In the mixing study, measurements are made of arrival times of fuel particles from the point of their injection (either at the top or near the bottom of the bed) to locations of two separate optical probes inside the bed. These arrival times, which are statistical quantities, are recorded simultaneously on two channels in both analog (stripchart) and digital form. Two quantitative mixing parameters have been defined and measured as a function of fluidization parameters. One of these is the first observed particle arrival time, t_o, after injection of a particle batch; this parameter measures the dispersal efficiency of particles from the injection location. The second mixing parameter is the average frequency of arrivals at probe i, $f_i = N_i/t$, where N_i is the number of arrival counts over the period t. This parameter gives a measure of circulation efficiency of particles at the location of probe i. It has been found that t_o and f_i are: (a) strongly affected by the gas fluidization velocity; (b) significantly affected by bed depth and location of optical probes in the bed; and (c) virtually unaffected by other fluidization parameters (temperature, oxygen content in gas, particle sizes) over the range of interest in fluidized-bed combustion. The measurements of t_o and f_i have resulted in definition of three mixing regimes, in terms of dimensionless fluidization velocities, U/U_{mf}: (a) good mixing throughout the bed; (b) no penetration of particles from the surface into the interior of the bed; and (c) an intermediate regime in which there is circulation of solids in the upper portions, but stagnation in lower portions of the bed.

Adsorptive and Desorptive Characteristics of Water Vapor Interacting with Polymer Composite Film for Humidity Sensing

P.H. Huang

Polymeric films have been used increasingly in solid state electronics as sensing elements for species concentration measurements in gases. The objective of this work is toward better understanding of the sorption and desorption isotherms of water vapor on a polymer composite film. The composite films of polyvinylchloride-styrenesulfonate have been investigated using the measured electrical conductance of the sensing film, at various frequencies, as a function of relative humidity at temperatures of 25, 50, and 90 $^{\circ}$C. A method is used to determine thermodynamic functions of the water vapor-polymer matrix interaction based on the measured conductivity data. This method of combined electrical and thermodynamic characterization of a gas/polymer system may be used to provide a means for designing suitable materials for gas sensing and may provide a method to model improved gas sensor behavior.

The experimentally determined entropy change on sorption/desorption is used to characterize and determine the degree of hysteresis occurring in the adsorbate/polymer system. The enthalpy change on sorption/desorption provides a direct measurement of the bonding state of adsorbates within the polymer composites and is used to characterize and determine the manner in which the adsorbed water molecules are bonded to specific sites in the polymer matrix. The free energy change on adsorption/desorption is used to represent the tendency of water vapor/polymer composite system for interaction. These thermodynamic functions have been obtained as a function of temperature, up to 90 $^{\circ}$C, at various relative humidities, in the range 5 to 97 percent, for a polymer composite film of polyvinylchloride-styrenesulfonate.

Evaluation of Relative Humidity Values for Saturated Aqueous Salt Solutions Using Osmotic Coefficient

P.H. Huang, J.R. Whetstone

The primary objective of this research is to provide a data base for relative humidity values in air in equilibrium at one atmosphere, for calibration of humidity sensors using saturated aqueous salt solutions. There is an increasing need for science and industry to provide a wide range of constant relative humidity values at elevated temperatures using saturated salt solutions. The thermal properties of aqueous electrolytes (such as the apparent molal heat capacity, and the relative apparent molal enthalpy as a function of molality up to saturation) required to obtain relative humidity values, are very limited in the literature and appear to be available only for sodium chloride and potassium chloride solutions. Experimental data on water vapor pressure, for most of the saturated salt solutions, are not available at temperatures up to 100 °C.

We have recently used a new method to evaluate the values of relative humidity in air, at one atmosphere, for eighteen saturated and stable uni-univalent, uni-bivalent, and bi-univalent water-saturated salt solutions. The method has accurately represented correlating equations for the osmotic coefficient, and experimentally determined osmotic coefficient values for the systems at 25 °C. A form of the Weiss equation is used to fit values of the saturated salt solutions molalities up to a temperature of 100 °C. Corrections for the nonideality of water vapor are made. The results for saturated aqueous sodium chloride solutions are compared with those obtained from a rigorous thermodynamic method.

Tables have been provided for relative humidity values of eighteen saturated salt solutions of sodium chloride, sodium fluoride, ammonium chloride, lithium chloride, potassium chloride, sodium nitrate, potassium nitrite, sodium nitrite, barium chloride, strontium chloride, cobalt bromide, nickel chloride, nickel nitrate, lithium sulfate, potassium sulfate, sodium carbonate, sodium sulfate, and potassium carbonate. The salts cover the range from approximately 3 to 97 percent relative humidity over the temperature range 50 to 100 °C. Also included are associated solubilities, osmotic coefficients, and Gibbs energies of water in the solutions. Maximum errors of the evaluated osmotic coefficients and relative humidity values are also provided.

Thin Film Thermocouples

K.G. Kreider

Thin film sensors are being investigated which will permit improved temperature and composition measurement in chemical process streams. Thin film thermocouples can provide dramatic improvements in response and accuracy for measuring temperatures in process streams. The DoE sponsored work on high temperature gas turbine thermocouples has been published, and emphasis is now being placed on thin film thermocouples for diesel engine combustion chambers. Present activities include an investigation of the feasibility of using new base metal systems on alumina and partially stabilized zirconia, and development of adhesion enhancers between the precious metal thermocouples and the ceramic hardware materials. The new sputtered film systems include the nisil-nicrosil bimetallic system, which has the highest temperature capabilities of any base metal system, and chromel-constantan, which has the highest output.

Large thermocouple arrays (20x20 cm) have been produced using type E (chromel-constantan) sputtered alloys on polyimide film. These arrays are capable of determining average temperatures of large areas involved in heat transfer, such as windows, with minimal perturbation of the convective heat transfer. The arrays can also simultaneously measure temperature distribution over large areas.

Thin Film Sensors

K.G. Kreider

Tin oxide and iridium tin oxide (ITO) films are being investigated as transparent electrical conductors. These films can be produced with excellent transparency and still exhibit useful conductance (10^{-4} cm/ohm) for heat generation. The Army is interested in these films for decontamination. By tailoring the Fermi level of the intermetallic oxide, exceptional optical and electrical properties can be realized. Other oxides investigated for their electrical/optical properties include ZrO_2 and Ta_2O_5. The sputtered films have unique structural characteristics and can be produced in amorphous, metastable, or equilibrium forms. X-ray, ellipsometry, and four point probe tests are used to monitor the properties.

Because of its unique capabilities for producing films, the RF planar magnetron has been used to produce quasi-crystals. The first experiments have been used to relate the fabrication temperature and annealing temperatures to the X-ray structure of the aluminum-manganese system. This system has unusual electrical, magnetic, and structural characteristics. By precisely controlling the substrate temperature during sputter deposition, the first icosahedral quasi-crystals were produced by film deposition. Competition between the amorphous, Al_6Mn, icosahedral, Al_4Mn, and T(dodecahedral) phases was monitored using X-ray diffraction on alloys with 30 weight percent Mn.

Iridium oxide thin films are being studied as chemical sensors based on their pH response. A study of the materials for pH sensing related to nuclear waste containment was published for the Nuclear Regulatory Commission. The relationship between the fabrication, structure, and properties of sputtered IrO_2 films is also being studied. The transition from amorphous to crystalline IrO_2 (rutile) was documented (J. Vac. Sci.) and related to the electrical conductivity. This structural definition appears to be a critical point in explaining previously published contradictory results on ion interferences and stability.

Chemical Sensor Research

S. Semancik, D. Cox

Contact sensors can detect and quantify a variety of chemical species, and they are therefore of potential use in a large number of process control applications. However, for these devices to reach their fullest utility, certain performance shortcomings that now exist must be overcome. The most serious problems are connected with attaining desired levels of selectivity and reproducibility in the sensor measurements. Dealing with these inadequacies requires a deeper understanding of the fundamental interactions that occur between the sensor and its environment.

In essentially all cases, the species being monitored adsorbs on the active film of the sensor and produces a change that affects both the interface chemistry and the physical properties of the film. It is from these changes that a measurable signal is derived (e.g., a change in conductance produces a lower current flow through the device). In order to understand the mechanisms which relate the chemical effects and physical responses within the sensing film element, a special combination of techniques is being assembled into a single apparatus in the Process Sensing Group.

The main dual chamber vacuum system for this apparatus was installed at NBS during May 1985. Components were fitted for X-ray and ultraviolet photoemission, and a small spot ion gun was mounted which will be used in ion scattering measurements. These techniques have been fully tested and are now operational. The computer-based data acquisition and control equipment for the facility has also been installed. A gas handling system was designed and constructed within the Group, and connected to the vacuum enclosure, to provide pure gases and gas mixtures to simulate different environmental ambients. A vibrating reed capacitance probe was procured for monitoring film work-function changes, and arrangements were made to assemble hardware that will be used to study substrate and overlayer structural factors. Installation of these components and a specially designed mass spectrometer is expected in the early part of 1986.

This new facility will permit changes in composition and stoichiometry, produced by adsorption, to be monitored in a variety of sensing materials. More importantly, these effects will be directly correlated with electronic sensing measurements made within the same system and on the same model substrates. Work thus far has been focused on the interaction between water vapor and oxide surfaces. Initial results for tin oxide (SnO_2), a semiconducting material widely applied in gas sensing applications, have demonstrated that the structure and adsorption chemistry of tin oxide is strongly dependent on the annealing temperatures at which it is treated.

(These findings are of importance for determining the best conditions for fabricating tin oxide sensor films.) The adsorption of water has been observed to alter the work-function of the SnO_2 interface and cause band bending in the electronic structure of the near-surface region. Further investigation of these effects is expected to lead to a basic model, explaining conductivity changes produced by water on tin oxide. Such a model would be helpful for understanding the interference effects of moisture when SnO_2 is used to detect other species, as well as determining in what way SnO_2 might be most suitably used to measure moisture content.

5. HONORS AND AWARDS

Robert J. Santoro - Department of Commerce, Silver Medal for his research on the fundamental processes leading to particle formation in high temperature chemically reacting flows.

Andre Macek - Department of Commerce, Bronze Medal for his outstanding contributions to the science and technology of fluidized bed reactors.

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Semancik, S., Doering, D.L. and Madey, T.E., Summary abstract: the interaction of water with Li-predosed Ru (001), J. Vac. Sci. and Tech., Vol. A3, No. 3, pp. 1571-1572 (1985).

Smyth, K.C., Miller, J.H., Dorfman, R.C., Mallard, W.G. and Santoro, R.J., Soot inception in a methane/air diffusion flame as characterized by detailed species profiles, Combustion and Flame, Vol. 62, pp. 157-181 (1985).

7. TALKS

Mattingly, G.E., Fluid Metering Research at NBS: New Research Tools and New Opportunities, ISA 84 - Process Measurement and Control Division, Session on Flow Measurement, Houston, TX, Oct. 23, 1984.

Mattingly, G.E., Fluid Measurement Research - Prospects for Progress, Department of Mechanical Engineering, University of Houston, Houston, TX, Oct. 23, 1984.

Mattingly, G.E., Liquid Flowrate Calibration Techniques, International District Heating and Cooling Association (IDHCA) Workshop on District Cooling Systems, Washington, DC, Nov. 20, 1984.

Mattingly, G.E., A New Strategy for Determining Flowmeter Installation Specifications, ASME Research Committee on Fluid Metering, Winter Annual Meeting, New Orleans, LA, Dec. 4, 1984.

Mattingly, G.E., Fluid Flow Measurement - Devices, Calibrations, and Traceability, 1985 ASHRAE Winter Meeting, Chicago, IL, Jan. 27, 1985.

Mattingly, G.E., Flow Measurement - Devices, Calibrations, and Applications for Nuclear Industries, Seminar Program, Department of Chemical Engineering, Howard University, Washington, DC, Mar. 22, 1985.

Mattingly, G.E., Fundamentals of Flow Measurement, 31st International ISA Symposium, San Diego, CA, May 7, 1985.

Mattingly, G.E., Fluid Metering Research at NBS - New Research Tools and New Strategies, Flow Technology, Inc., Phoenix, AZ, May 8, 1985.

Mattingly, G.E., Air Flow Rate Measurements - Techniques, Calibrations, and Traceability, Center for Manufacturing Research and Technology Utilization and Department of Mechanical Engineering, Tennessee Tech. University, Cookeville, TN, May 28, 1985.

Mattingly, G.E., Standards for Thermal Metering, 1985 Annual Meeting of the International District Heating and Cooling Association (IDHCA), Minneapolis, MN, June 18, 1985.

Mattingly, G.E., Volume Flow Measurements, Fluid Mechanics Measurements Short Course, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN, June 21, 1985.

Bryner, N.P. (Coauthor: R.V. Calabrese), A Facility to Study Drop Breakup in the Vicinity of Simulated Mixer Elements, Mixing X, Engineering Foundation Conference, Henniker, NH, Aug. 5, 1985.

Ghosh, A.K. (Coauthor: J.J. Ulbrecht), Bubble Formation from Submerged Orifices in Flowing Liquids, Mixing X, Engineering Foundation Conference, Henniker, NH, Aug. 5, 1985.

Yuk, K.I. (Coauthor: J.J. Ulbrecht), Formation of Bubbles in Shear Flow from a Gas Filled Cavity, Mixing X, Engineering Foundation Conference, Henniker, NH, Aug. 5, 1985.

Calabrese, R.V. (Coauthor: P.D. Berkman), Drop Size Distributions Produced by Static Mixers, Mixing X, Engineering Foundation Conference, Henniker, NH, Aug. 5, 1985.

Mattingly, G.E., Preliminary Results for a Vortex-Induced Liquid Handling and Accountability Procedure at Zero Gravity, Helium Transfer in Space Workshop, NBS, Boulder, CO, Aug. 19-21, 1985.

Mattingly, G.E., Flow Measurement Assurance Programs - Round Robin Testing Strategies, Idaho National Engineering Laboratory, Idaho Falls, ID, Sept. 5, 1985.

Macek, A., Optical Measurements of Char-Particle Temperatures and Radiant Emissivities in Fluidized-Bed Combustors, 3rd International Fluidized Conference, London, England, Oct. 16, 1984.

Horvath, J.J., Flame Temperature Measurements in Premixed and Diffusion Flames by Collisional Redistribution of Laser Excited Levels, Sandia National Lab - Combustion Research Facility, Livermore, CA, Oct. 25, 1984.

Davis. R.W., Computer Simulations of Vortex Splitting and Vortex Merging using Time-Dependent Finite Difference Codes, 37th Annual Meeting of the Division of Fluid Dynamics, American Physical Society, Providence, RI, Nov. 18-20, 1984.

Ray, S.R. (Coauthor: R. Goulard), Optical Tomography in Combustion and Meteorology, Workshop on Advances in Remote Sensing Retrieval Methods, Williamsburg, VA, Oct. 30 - Nov. 2, 1984.

Semerjian, H.G., Soot Formation in Laminar Diffusion Flames, Seminar presented at the Johns Hopkins University, Department of Chemical Engineering, Baltimore, MD, Nov. 5, 1984.

Ray, S.R. (Coauthors: P.J. Emmerman and H.G. Semerjian), High Speed Laser Tomography in Flames, International Conference on Lasers '84, San Francisco, CA, Nov. 26-30, 1984.

Smyth, K.C. (Coauthors: J.H. Miller, W.G. Mallard and R.J. Santoro), Detailed Structure Studies of a Laminar Methane/Air Diffusion Flame I. Optical Measurements, presented at the Eastern Section Meeting: The Combustion Institute, Clearwater, FL, Dec. 3-5, 1984.

Semerjian, H.G., Optical Sensing in Chemical Reactors, NBS Staff Research Seminar, Gaithersburg, MD, Dec. 13, 1984.

Santoro, R.J., Particle Formation in Flames, NBS Staff Research Seminar, Gaithersburg, MD, Dec. 20, 1984.

Preston, R.E., Laser Spectroscopy of Single Levitated Droplets, NBS Staff Research Seminar, Gaithersburg, MD, Dec. 23, 1984.

Semerjian, H.G., Optical Diagnostics in Chemically Reacting Flows, Seminar presented at Lehigh University, Biotechnology Research Center, Bethlehem, PA, Jan. 25, 1985.

Santoro, R.J., Fuel Structure Effects on Soot Formation Processes, invited presentation at the Particle Emission Technology Meeting, Naval Postgraduate School, Monterey, CA, Apr. 16, 1985.

Lettieri, T.R. (Coauthors: R.E. Preston, H.G. Semerjian and S.R. Ray), Elastic and Raman Scattering from Evaporating Levitated Droplets, Sixteenth Annual Meeting of the Fine Particle Society, Miami, FL, Apr. 22-26, 1985

Santoro, R.J. (Coauthor: H.G. Semerjian), Laser Light Scattering Measurements of Soot Particles in Flames, Sixteenth Annual Meeting of the Fine Particle Society, Miami, FL, Apr. 22-26, 1985.

Horvath, J.J. (Coauthor: H.G. Semerjian), Temperature Measurements in a Diffusion Flame using Thermally Assisted Fluorescence, Conference on Lasers and Electro-Optics, Baltimore, MD, May 21-24, 1985.

Santoro, R.J. (Coauthors: T.T. Yeh and H.G. Semerjian), Laser Light Scattering Measurements of Soot Particles in Flames, Conference on Lasers and Electro-Optics, Baltimore, MD, May 21-24, 1985.

Ray, S.R. (Coauthor: H.G. Semerjian), High Speed Laser Tomographic Measurements in Fluctuating Flames, Conference on Lasers and Electro-Optics, Baltimore, MD, May 21-24, 1985.

Semerjian, H.G., Optical Techniques for Cell Activity and Concentration Measurements, Workshop on Process Measurements for Biotechnology, NBS/CCE, Gaithersburg, MD, May 29-30, 1985.

Semerjian, H.G. (Coauthors: C. Presser, A.K. Gupta and R.J. Santoro), Droplet Size Measurements in a Swirling Kerosene Spray Flame by Laser Light Scattering, International Conference on Liquid Atomization and Spray Systems, London, England, July 8-10, 1985.

Ray, S.R., Laser Tomography Technique for Simultaneous Measurement of Species Concentration and Temperature, Grumman Aerospace Corp., Bethpage, NY, June 19, 1985.

Macek, A., Fundamental Studies of Black Liquor Combustion, DoE Contractor's Meeting, Orono, ME, July 30, 1985.

Santoro, R.J. (Coauthors: T.T. Yeh and H.G. Semerjian), The Transport and Growth of Soot Particles in Laminar Diffusion Flames, AIChE/ASME National Heat Transfer Conference, Denver, CO, Aug. 4-7, 1985.

Macek, A., Characterization of Solids Mixing in a Laboratory-Scale Fluidized Bed, DoE Advanced Research and Technology Development Conference, Morgantown, WV, Aug. 14, 1985.

Davis, R.W., Numerical Modeling of Unsteady Shear Flows, Computational Aerodyamics Group, Wright-Patterson AFB, Dayton, OH, Sept. 1985.

Santoro, R.J., Soot Particle Formation Processes in Flames, Advanced Fuels Research, Hartford, CT, Oct. 4, 1985.

Hasegawa, S., Some Performance Characteristics of Hygrometers for Energy Management Control System Applications, ASHRAE Seminar, Chicago, IL, Jan. 27, 1985.

Hasegawa, S., National Basis of Accuracy in Humidity Measurements, Int'l. Symp. on Moisture and Humidity, Washington, D.C., Apr. 15, 1985.

Hasegawa, S. and Hurley, C.W., Humidity Sensors for HVAC Applications, Recent Advances in Control and Operation of Building HVAC Systems, Int'l. Symp., Trondheim, Norway, May 23, 1985.

Cox, D.F. (Coauthor: Hoflund, G.B.), ELS Characterization of Tin Oxide Surfaces, American Physical Society National Meeting, Baltimore, MD, Mar. 27, 1985.

Huang, P.H. and Whetstone, J.R., Evaluation of Relative Humidity Values for Saturated Aqueous Salt Solutions Using Osmotic Coefficients between 50 and 100 $^{\circ}$C, Int'l. Symp. on Moisture and Humidity, Washington, D.C., Apr. 16, 1985.

Huang, P.H., Electrical and Thermodynamic Characterization of Water Vapor/Polymeric Film System for Humidity Sensing, Third Int'l. Conf. on Sensors and Actuators, Philadelphia, PA, June 11, 1985.

Semancik, S. (Coauthors: Doering, D.L. and Madey, T.E.), The Interaction of Water with Li-Predosed Ru(001), 31st National Symposium of the American Vacuum Society, Reno, NV, Dec. 5, 1984.

Semancik, S., An Overview of the Third International Conference on Solid-State-Sensors, NBS/CCE, Chemical Process Metrology Div. Seminar, Gaithersburg, MD, June 26, 1985.

Semancik, S. (Coauthor: Cox, D.F.), Factors Influencing the Chemistry of Tin Oxide Surfaces, Third Int'l. Conf. on Solid State Sensors and Actuators, Philadelphia, PA, June 14, 1985.

Semancik, S., The Influence of Alkali Additives on H_2O-Metal Interactions, Gordon Conference on Chemistry at Interfaces, Meriden, NH, July 23, 1985.

Whetstone, J.R., Development of Basic Orifice Discharge Cofficients, 64th Annual Gas Processors Association Conf., Houston, TX, Mar. 18-20, 1985.

Whetstone, J.R., Development of Basic Orifice Discharge Coefficients, Meeting of ISO Technical Committee 30, Subcommittee 5, Tokyo, Japan, Nov. 13, 1984.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

J.J. Ulbrecht

National Research Council - Committee on Bioprocessing for the Energy Efficient Production of Chemicals (Liaison Representative)
National Research Council - Bioengineering Systems Research Panel (Liaison Representative)
AIChE National Programs Committee - Area 3a Mixing (Vice Chairman)
AIChE International Activities Committee (Member)
ASTM Biotechnology Committee (Member)

G. Kulin

ASTM D.19, Main Committee on Water (Member)
- Task Group D19.03.03.02 on Velocity Measurements (Chairman)
- Task Group D19.03.03.03 on Velocity-Area Methods (Chairman)
- Task Group D19.03.03.08 on Measurement of Small Flows (Chairman)

G.E. Mattingly

ASME (Main) Committee on the Measurement of Fluid Flow in Closed Conduits (Member)
ASME SC-2, Pressure Differential Devices (Member)
ASME SC-6, Glossary of Terms for Flow Measurements (Chairman)
ASME SC-14, Measurement of Fluid Flow Using Gravimetric and Volumetric Techniques (Chairman)
ASME SC-15, Committee on Vortex Shedding Type Flowmeters (Chairman)
ASME SC-16, Committee on Installation Requirements for Orifice, Venturi, and Nozzles (Member)
ASME (Main) Research Committee on Fluid Meters (Member)

ASME SC-11, Test Methods and Calculation Procedures (Chairman)
ASME Ad Hoc Committee on Flowmeter Installation-Effects Research (Member)
International District Heating Association (IDHA) Fluid Metering Committee (Member)

N.E. Mease

ASTM D0.22, Methods of Sampling and Analysis of Atmospheres (Member)
ASTM SC.02, Methods of Sampling and Analysis (Member)
ASTM SC.05, Calibration (Member)
ASTM SC.11, Meteorological Measurement (Member)

A. Macek

Combustion Institute - 21st Symposium (International) on Combustion, Program Subcommittee (Member)

R.J. Santoro

Combustion Institute
21st Symposium (International) on Combustion
Program Subcommittee (Member)
Publications Committee (Member)
Eastern States Section - Papers Chairman

H.G. Semerjian

Combustion Institute
21st Symposium (International) on Combustion
Program Subcommittee (Member)
ASME Heat Transfer Division, K-11 Committee on Heat Transfer in Fires and Combustion Systems (Member)
AIChE Engineering Sciences and Fundamental Group, Area 1b - Kinetics, Catalysis and Reactor Engineering (Member)
AIChE Food, Pharmaceutical and Bioengineering Division, Area 15C Biotechnology (Member)
NBS Research Advisory Committee (Chairman)

S. Hasegawa

ASME PTC 19.18, Committee on Humidity Determination (Member)
ASTM D22, Sampling and Analysis of Atmospheres (Member)
ASTM D22.11, Meteorology (Subcommittee Vice Chairman)
ASTM G3, Durability of Nonmetallic Materials (Member)
Program Committee, International Symposium on Moisture and Humidity (Member)

K.G. Kreider

Advisory Panel, Center for Chemical Electronics, U. of PA (Member)
ASTM E20, Temperature (Member)
ASTM C30, Composite Materials (Member)
Program Committee, Int'l. Conf. on Solid State Transducers (Member)
Steering Committee on 1985 Int'l. Symp. on Moisture and Humidity (Member)

F.E. Jones

ANSI/INMM Writing Group on Tank Volume Calibration (Consultant)

EDITORSHIPS

G.E. Mattingly

International Journal of Heat and Fluid Flow (Editorial Advisory Board)

A. Macek

Combustion Science and Technology (Editorial Advisory Board)

9. PROFESSIONAL INTERACTIONS

FACULTY APPOINTMENTS

J.J. Ulbrecht

Adjunct Professor, Department of Chemical Engineering, University of Maryland.

INDUSTRY

K.R. Benson

Consultation with A. Johnson of Douglas Aircraft regarding mass vs. volume flow calibrators.

Consultation with R. Kim of Babcock & Wilcox regarding new gas flow meter and calibration techniques.

Consultation with W. Scavuzzo of Eris Medical Technologies regarding air flow rate for pulmonary function.

Consultation with K. Westerson of Cummins Engine regarding hydrometer calibrations and use; effects of varnish build-up in glass tube variable area meters.

Consultation with Mr. Beam of Krohne-America regarding standards for correlating their new U.S. facility with the parent Dutch facility.

Consultation with Mr. Cassiole of U.S. Testing Co. regarding orifice testing standards and techniques.

Consultation with J. Sawyers of CME, Inc. regarding calibration of laminar transfer references for Saudi Arabia.

Consultation with P. Pringle of Max Machinery regarding correlation using positive displacement flow meters.

Consultation with E. Uses of General Electric Co. regarding mass flow meter correlation and calibration techniques for in-flight refueling.

Consultation with J. Kerwin of Lockheed-Lemsco regarding sonic nozzle calibration and use as a transfer standard.

Consultation with D. Ruffner of Ametek regarding calibration of liquid flow nozzles as a transfer standard for Saudi Arabia.

Consultation with W. Fling of Cities Service Oil & Gas regarding API Orifice Tests.

Consultation with S. Caldwell of Colorado Engineering Experiment Station regarding gas flow calibration with laminar meters and sonic nozzles.

Consultation with T. Kendzior of Pratt and Whitney regarding turbine meter calibration and interlab correlation.

Cooperative research with R. Peele of Corning Glass Works regarding nitrogen flow by characterizing laminar meter performance as a transfer standard.

Cooperative research with J. Bloom of Flo-Tron, Inc. regarding ascertaining accuracy of new mass flow calibrator for hydrocarbon liquids.

Cooperative research with P. Twigg of Westinghouse Electric Corporation regarding ascertaining accuracy of laminar flow with nitrogen for AWAC aircraft.

Cooperative research with R. Shafer of Aberdeen Proving Ground regarding a leakage rate standard for gas mask valves.

A.K. Gaigalas

Collaboration with Institute of Paper Chemistry, Appleton, WI, for testing of pulp consistency meter in the IPC pulp loop.

G.E. Mattingly

Consultation with B. Kamentser and C. Watson of ITT-Barton on theories for vortex shedding flow meter flowfields.

Consultation with P. Brooks of United McGill Corporation regarding design considerations for special "in-situ" flowmeter proving device.

Consultation with M. Miller of Talley Defense Systems regarding design and construction of low air flow calibration facility.

Consultation with C. Vaughn and G. Mallet of General Electric regarding in-situ flow meter calibrations.

Consultation with J.A. Hicks of American Gas Association regarding Conference on Flow Measurement scheduled for November 1986.

Consultation with M. Reischman (ONR), G. Lea (NSF), J. Hanson and E. Hendricks (NRL), and S. Deutsch and C. Merkle (Pennsylvania State University) on NBS water tunnel research.

Consultation with G. Bankoff, Department of Chemical Engineering, Northwestern University, on two-phase flow research in the NBS water tunnel.

Consultation with ASME's two committees on fluid metering - MFFCC and the Research Committee for Fluid Metering, on the NBS slurry flow loop.

Consultation with L.P. Purtell, USN - DTNSRDC, on wind tunnel testing programs to measure separated flow on submarine hulls.

N.E. Mease

Consultation with E. Brady of General Dynamics, Convair Division, regarding special instrument calibration for FAA and performance specification of General Dynamics wind tunnel.

Consultation with D. Bevan of Boeing/Vertol regarding special calibration test on wind tunnel instruments.

Consultation with R. Roberge, Environmental Instruments, Inc., regarding specialized product testing and generation of basis for military bid certification.

Consultation with F. Hagen, Rosemount, Inc., regarding specialized product testing and generation of basis for military bid certification.

Consultation with D. Mahoney, Freedona Development Co., regarding measurements of compressed air flow.

B. Robertson

Consultations with a group of vortex-shedding flowmeter manufacturers and users.

S.R. Charagundla

Collaboration with P. Ariessohn, Weyerhaeuser Co., on emission measurements in recovery boilers.

Collaboration with R. Barreis and D. Smiley of Champion International on emission measurements in recovery boilers.

A. Macek

Cooperative work with R. Corbeels of Texaco Research on combustion of coke particles in fluidized beds.

A. Macek and H.G. Semerjian

Collaboration with R. Coates of Mountain Fuel Resources on diagnostics in high pressure entrained flow gasifiers.

Collaboration with E. McHale and M. King, Atlantic Research Corp., on slurry combustion.

S.R. Ray

Consultations with R. Oman of Grumman Aerospace on application of laser tomography for diagnostics in gas turbine engine plumes.

R.J. Santoro and S. Semancik

Consultation with T. Baker of Exxon Research on coke formation on catalytic surfaces.

R.J. Santoro and H.G. Semerjian

Collaboration with S. Harris, General Motors Research Laboratories, on soot particle nucleation.

R.J. Santoro and H.G. Semerjian

Collaboration with P. Solomon of Advanced Fuel Research on temperature measurements in diffusion flames.

H.G. Semerjian and S.R. Ray

Collaboration with P. Solomon of Advanced Fuel Research on laser tomography.

H.G. Semerjian

Consultation with J.D. Jobe and T. Schmidt of Shell Development on measurements in high temperature reactors.

Consultations with P. Girling of Air Products Company on temperature measurements in CVD furnaces.

Consultations with R. Seeker of Energy and Environment Research on combustion of hazardous wastes.

S. Hasegawa

Consultation with J. Steichen of DuPont on low humidity generator.

Consultation with G. Turk and F. Mermoud, Liquid Air - U.S. and France, on low humidity measurements, generation, and calibration.

Consultation with J. Pernicka of Pernicka Corporation on humidity measurements and standards which are applicable for semiconductor packages.

Consultation with L. Woody of Bell South and G. Truesdale of Raychem on measurement and control of humidity in telephone pedestals.

F.E. Jones

Consultation with DuPont staff on tank volume calibration.

ACADEME, NATIONAL LABORATORIES, AND GOVERNMENT

K.R. Benson

Consultation with D. Todd of the North Island (CA) Naval Air Station regarding bell-prover volume vs. dynamic errors, and laminar meter and sonic nozzle transfer standards.

Consultation with H. Stump, NASA Langley Research Center, regarding mass flow of gas/liquid two phase flow for space station.

Consultation with V. van der Pluym of South African Bureau of Standards, Pretoria, regarding calibration laboratory for large water pumps.

Consultation with H. Whitzel of U.S. Naval Ship Research and Development Center regarding ultrasonic flow meters for secondary in-situ calibration for nuclear submarine applications.

Cooperative research with A. Szilvassy, National Office of Measures, Budapest, Hungary, regarding turbine meter use in standard transfer correlation.

A.K. Gaigalas

Collaborative research initiated with R.V. Calabrese of the University of Maryland on ultrasound techniques for cell concentration measurement.

G. Kulin

Served on National Science Foundation sub-panel for evaluation of engineering-center proposals, Nov. 8-9, 1985.

S. Semancik

Served on National Science Foundation Evaluation Panel on Catalysis.

G.E. Mattingly

Cooperative research with A. Szilvassy, National Office of Measures, Budapest, Hungary, on NBS-Gaithersburg metering cross-check program, Sept. 23-30, 1985.

Consultation with J.M. Hobbs of NEL/UK on NBS-Gaithersburg orifice metering cross-check program.

Consultation with R.C. Mottram, University of Surrey, Guildford, UK, on pulsation effects on flowmeters.

Consultation with K. Yoshida, National Research Laboratory of Metrology, Japan, on Flowmeter Calibration Techniques and Interlaboratory Testing.

Consultation with P. Fahlen of National Testing Institute, Sweden, on flow measurements for heat pump systems.

Consultation with A.B. Chesnoy and R. Quin, Total, France, and M.J. Bosio and K. Killerud, Statoil, Norway, on petroleum proving techniques and design of planned station for North Sea Products.

Consultation with Y.P. Lin, Taiwan Institute of Standards on flow measurement standards.

Consultation with G. Liu, Taiwanese Coord. Council for North American Affairs, regarding flow measurement standards, calibration facilities, and traceability.

Consultation with J.S. Bodner, Scientific and Technical Affairs Officer, American Embassy, Budapest, regarding flow measurement capabilities at NBS-Gaithersburg.

Consultation with N.A. Khan, Pakistani Council for Scientific and Industrial Research, on fluid measurement calibration and research facilities.

Consultation with P. Wolfs, N.V. Nederlandse Gas Unie, regarding gas flow rate measurement techniques and research tools.

Consultation with G. Maoxiang, China Ship Scientific Research Center, Shanghai, regarding vortex shedding flow meter and flow meter installations-effects research at NBS-Gaithersburg.

Consultation with J. Smid, N.V. Nederlandse Gas Unie, regarding flowmeter installations-effects research.

Consultation with D. Smith of NEL/UK regarding NEL-NBS orifice cross-check program.

Consultation with N. Veloz of the U.S. National Park Service on two-phase (walnut shells in air) flow measurement for use in cleaning statues.

Consultation with K. Biss, Bergen County (NJ) Prosecutor's Office, regarding assessment of flowmetering unit involved in a fatal fire.

N.E. Mease

Consultation with A. Cohen of U.S. Bureau of Mines on the effects of turbulence on mean speed anemometer indications.

Consultation with B. Mahajan of the NBS/CBT Building Equipment Division on specialized calibrations for instruments for ventilation research.

Collaborative research with E. Simiu of the NBS/CBT Structures Division on measurements to specify wind-based aeroelastic loadings on structures.

Consultation with W. Saric of Arizona State University on the characteristics of fluctuating flows in wind tunnels.

B. Robertson

Collaboration with B. Tribollet of the Centre National de la Recherche Scientifique, Paris, France, on experimental electrochemical techniques for measuring mass transfer and shear stress in liquids.

Consultation with C. Deslouis of the Centre National de la Recherche Scientifique, Paris, France, on theory of diffusion measurements by electrochemical means.

Consultation with A.E. Humphrey of Lehigh University on diffusion measurement in gels and shear rate measurement in broths.

Consultation with R.V. Calabrese of University of Maryland on shear rate measurements on stirrer blade in mixing tanks.

J.R. Whetstone

Collaboration with D.S. Loebbaka of the University of Tennessee (Martin) on X-ray tomography for slurry flow solid fraction measurements.

S.R. Charagundla

Consultations with G.L. Pellett of NASA Langley Research Center on microencapsulation technology.

Collaborative effort initiated with B. Northram of NASA Langley Research Center on fiber optics sensing techniques.

R.W. Davis

Collaboration with M. Kurosaka of MIT, Department of Aeronautics and Astronautics, on computation of massless particle paths through bluff body wakes for comparison with his experimental data for turbomachinery.

Consultation with C.A.J. Fletcher, University of Sydney, Department of Mechanical Engineering, Sydney, Australia, on computation of vortex shedding from square cylinders, which will be included in a forthcoming book.

R.W. Davis and R.J. Santoro

Collaborative research with H. Baum of the NBS Center for Fire Research on numerical modeling of chemically reacting flows.

J.J. Horvath

Consultation with C. Proctor of University of Florida on thermally assisted fluorescence measurements.

Consultation with W. Lempert of NASA Langley Research Center on laser-excited fluorescence techniques for temperature measurements in scram jets.

Consultation with J. Dec of Sandia National Laboratories on temperature measurements in a pulsed combustor.

Consultation with S. Weeks of Ames Laboratory, Iowa State University, on ultrasonic nebulization of liquids.

A. Macek

Collaborative research with W. Liggett of the NBS Center for Applied Mathematics on statistical analysis of mixing processes in fluidizing beds.

Collaborative research initiated with D. Smoot of Brigham Young University, Chemical Engineering Department, on diagnostics in entrained flow gasifiers.

Collaborative research with D. Shaw of Ohio State University on mixing studies in fluidized beds.

Planning of cooperative DoE/NBS projects with DoE Morgantown Energy Technology Center on coal gasifier diagnostics; discussions of on-going and future fluid-bed measurements.

C. Presser and H.G. Semerjian

Collaborative research with A. Gupta of University of Maryland on diagnostics in spray flames.

S.R. Ray

Collaborative research with D. Orser of the NBS Center for Applied Mathematics on three-dimensional graphics for laser tomography.

S.R. Ray and H.G. Semerjian

Collaborative research with R. Goulard of George Washington University on laser tomography.

R.J. Santoro and H. G. Semerjian

Cooperative research with R.A. Dobbins of Brown University on interpretation of optical measurements of particles in flames.

Collaborative research with H. Hayasaka of Hokkaido University, Japan, on studies of temperature effects on soot formation processes.

Collaborative research with K. Smyth and W.G. Mallard of the NBS Center for Fire Research on particle formation in high temperature reacting flows.

Cooperative research with D. Santavicca of Pennsylvania State University on Raman temperature measurements in particle laden flames.

H.G. Semerjian

Collaborative research being developed with J. Gentry of University of Maryland on investigation of levitated droplets.

Consultations with V. Hlavacek of State University of New York (at Buffalo) on heterogeneous reactions and chemical vapor deposition.

Collaborative research with S. Sikdar of the NBS Center for Chemical Engineering (Boulder) on concentration measurements in bioseparation systems.

Consultations with P. Ostrowski of Naval Surface Weapons Center on diagnostics in liquid spray systems.

H.G. Semerjian and J.J. Horvath

Collaborative research initiated with A.E. Humphrey and J. Phillips of Lehigh University on optical sensing in bioreactors.

H.G. Semerjian and A. Macek

Cooperative research with D. Clay of the Institute of Paper Chemistry on black liquor combustion and pyrolysis.

Cooperative research initiated with I. Stockel of University of Maine on droplet formation and black liquor combustion.

H.G. Semerjian and C. Presser

Cooperative work with J. Bellan and M. Clayton of JPL on diagnostics and modeling in spray combustion.

Cooperative research with D. Butler of Los Alamos Scientific Laboratories on modeling of spray flames.

Cooperative research being developed with J.Katz of Johns Hopkins University on temperature and particle measurements in high temperature reacting flows.

Consultations with R. Chawla of Howard University on combustion of hazardous wastes.

S. Hasegawa

Collaboration with staff of EG&G-Idaho and W. Gamill of Nuclear Regulatory Commission on generation and measurement of high humidity at elevated temperatures.

Consultation with J. Facundo of National Weather Service on specifications for testing radiosonde humidity sensors.

Consultation with R. Wylic of CSIRO (Australia) on the World Meteorological Organization's standard hygrometer.

Consultation with Y. Dazhi of Chang Chun Meteorologial Instrument Institute (China) on humidity generators.

F.E. Jones

Collaboration with B.E. Welch of the NBS Center for Basic Standards on improvement of pressure standards at the ppm level.

Consultant to the ANSI/INMM Writing Group on tank volume calibration.

S. Semancik

Collaboration with Professor D.L. Doering, Department of Physics, University of Florida, on coabsorption of Li and H_2O on Ru.

Collaboraton with T.E. Madey, NBS Surface Science Division on the effects of additives on surface reactions.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

Session on Fluid Measurements for Thermal Metering; International District Heating and Cooling Association (IDHCA) Workshop on District Cooling Systems, Washington, DC, Nov. 19-20, 1984. Co-chaired by G.E. Mattingly.

WORKSHOPS

Hosted industry-government consortium meeting on Vortex Shedding Flowmeter Research at NBS, Gaithersburg, MD, Mar. 28, 1985. Organized by G.E. Mattingly.

Hosted industry-government workshop on Flowmeter Installation, Gaithersburg, MD, Apr. 22, 1985. Organized by G.E. Mattingly.

Hosted workshop on On-Line Measurement of Rheological Properties, Gaithersburg, MD, May 2-3, 1985. Organized by J.J. Ulbrecht.

Hosted workshop on Process Measurements for Biotechnology, Gaithersburg, MD, May 29-30, 1985. Organized by J.J. Ulbrecht.

Cosponsored workshop on Standardization Problems in the Design and Scale Translation of Bioreactors, held at Lehigh University, Bethlehem, PA, June 17-18, 1985. Organized by J.J. Ulbrecht and A.E. Humphrey.

Hosted NBS-DOE workshop on Two-Phase Flow Fundamentals, Gaithersburg, MD, Sept. 22-27, 1985. Organized by G.E. Mattingly.

Hosted workshop on Heat Meters (jointly with DOE and the International Energy Agency), Jan. 31-Feb. 1, 1985. Organized by G.E. Mattingly.

Session on Fluid Meters at ASME Winter Annual Meeting, New Orleans, LA, Dec. 9-14, 1984. Chaired by G.E. Mattingly.

NBS Staff Research Symposium on Aerosol/Particle Research, NBS, Gaithersburg, MD, Dec. 20, 1984. Organized and chaired by H.G. Semerjian.

SEMINARS

T. Papanastasiou, Department of Chemical Engineering and Materials Science, University of Michigan, Ann Arbor, MI: Modeling of Viscoelastic Flow, Dec. 12, 1984.

A.E. Humphrey, Center for Biotechnology Research, Lehigh University, Bethlehem, PA: Modelling and Design of Bioreactors, Oct. 4, 1984.

J.A. Phillips, Center for Biotechnology Research, Lehigh University, Bethlehem, PA: Problems in Monitoring Bioreactor Systems, Oct. 4, 1984.

T. Lindt, Department of Metallurgical and Materials Science, University of Pittsburgh, PA: Interaction Between Polymerization and Flow in Reactive Processing of Polymers, Mar. 20, 1985.

G.B. Tatterson, Department of Chemical Engineering, Texas A&M University, College Station, TX: Sound Spectra of Gas Dispersion in Agitated Tanks, Apr. 12, 1985.

G.B. Tatterson, Department of Chemical Engineering, Texas A&M University, College Station, TX: Image Processing of Flow Visualization Films, Apr. 12, 1985.

J. Wu, College of Marine Studies and Department of Civil Engineering, University of Delaware, Newark, DE: Two Phase Flow Measurement Techniques - Development and Use for Liquid Droplets in Gases and Bubbles in Liquids, Apr. 19, 1985.

C. Deslouis, Physique des Liquides et Electrochimie, Associe a l'Universite Pierre et Marie Curie, Paris, France: Transport Properties in Flowing Fluids by Electrohydrodynamic and Diffusion Impedances, May 20, 1985.

M. Lessen, University of Rochester, Rochester, NY: Instability and Turbulent Mixing in Jets and Other Geometries, May 23, 1985.

J.M. Hobbs, National Engineering Laboratory, East Kilbride, Glasgow, Scotland: Flow Measurement at NEL (U.K.): Calibrations, Research, and Traceability, May 28, 1985.

M.E. Ryan, Department of Chemical Engineering, State University of New York, Buffalo, NY: Melt Deformation and Heat Transfer in Injection Blow Molding, June 21, 1985.

G. Andrews, Department of Chemical Engineering, State University of New York at Buffalo, Buffalo, NY: Fluidized Bed Fermenters: Effect of Rheology on Design, July 10, 1985.

R.C. Mottram, Department of Mechanical Engineering, University of Surrey, England: Pulsation Effects on Vortex Meters, Aug. 9, 1985.

F.J. Bonner, Department of Chemical Engineering, Vanderbilt University, Nashville, TN: The Effect of Ultrasound on Suspension Polymers, Aug. 15, 1985.

X.B. Reed, Department of Chemical Engineering, University of Missouri-Rolla, Rolla, MO: Turbulence in Two-Phase and Chemically Reacting Systems, Aug. 27, 1985.

A.E. Humphrey and J.A. Phillips, Center for Biotechnology Research, Lehigh University, Bethlehem, PA: A Short Course on Bioreactor Design and Instrumentation, Twelve Lectures, Sept. 4, 18, Oct. 2, 16, Nov. 6, 20, 1985.

P.R. Solomon, Advanced Fuel Research, Inc., E. Hartford, CT: Measurement of Particle, Soot and Gas Temperature in Combustion using FTIR, Oct. 22, 1984.

V. Hlavacek, Chemical Engineering Department, State University of New York at Buffalo, Amherst, NY: High Temperature Self Propagating Synthesis of Refractory Materials, Nov. 20, 1984.

A. Gomex, Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ: Comparative Study of the Sooting Behavior of an Aromatic vs. Aliphatic in Diffusion Flames, Mar. 7, 1985.

K.F. Wall, Applied Physics Department, Yale University, New Haven, CT: Low Frequency Light Scattering from Roughened Silver Surfaces, Mar. 11, 1985.

S.L. Chung, Chemical Engineering Department, The Johns Hopkins University, Baltimore, MD: The Counterflow Diffusion Flame Burner: A New Tool for the Study of the Nucleation of Refractory Compounds, Mar. 14, 1985.

R. Joklik, Mechanical Engineering Department, University of California, Berkeley, CA: A Spectroscopic Study of the CH Radical in a Low Pressure Oxy/Acetylene Flame, May 31, 1985.

R.W. Pitz, General Electric Research and Development Center, Schenectady, NY: Laser Measurements in Jet Diffusion Flames, June 14, 1985.

W. Bartok, Exxon Research and Engineering Co., Annandale, NJ: Formation of Soot and its Precursors in Diffusion Flames, July 11, 1985.

Y. Tambour, Department of Aeronautical Engineering, Technion-Israel Institute of Technology, Haifa, Israel: A Lagrangian Sectional Approach for Simulating Droplet Size Distribution of Vaporizing Fuel Sprays in a Turbulent Jet, Sept. 20, 1985.

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Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1985 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science. They embody: development and improvement of measurement principles, measurement standards, and calibration services such as volumetric and mass flow rates, liquid volume, liquid density, and humidity; generation (via accurate measurement and advanced predictive models) of reliable reference data for thermophysical properties of pure fluids, fluid mixtures, and solids of vital interest to industry; and development of improved correlations, models, and measurement techniques for complex flows, heat and mass transport, mixing, and chemically reacting flows of interest in modern unit operations.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

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