NBSIR 84-3019

Center For Chemical Engineering

Technical Activities: Fiscal Year 1984

February 1985

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

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Center For Chemical Engineering Technical Activities: Fiscal Year 1984

J. Hord, Editor

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Boulder, Colorado 80303

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National Research Council (NRC)
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February 26-28, 1985
Boulder, Colorado

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Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1984 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, volume, 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 solid-fluid slurry 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 1984 (October 1, 1983 through September 30, 1984). This Center is one of six such units that comprise 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 a broad segment of American industry known as the Chemical Process Industry (including chemical, petrochemical, petroleum, paper, biochemical, food and drug, etc.). The goal of the Center is to provide measurement and data bases that assure equity in domestic and international trade; enable improved innovation, design, and control of chemical processes; and strengthen the competitiveness of U.S. industry in the world market.

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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- Applied Mathematics
- Electronics & Electrical Engineering
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering

CENTER FOR MATERIALS SCIENCE

- Inorganic Materials
- Fracture & Deformation
- Polymers
- Metallurgy
- Reactor Radiation

INSTITUTE FOR COMPUTER SCIENCES & TECHNOLOGY

- Programming Science and Technology
- Computer Systems Engineering

NATIONAL MEASUREMENT LABORATORY

- Basic Standards
- Radiation Research
- Chemical Physics
- Analytical Chemistry

ORGANIZATION OF THE CENTER FOR CHEMICAL ENGINEERING

CENTER FOR CHEMICAL ENGINEERING
*J.Hord, Director
M. Hessel, Deputy Director

***Chemical Engineering Science Division**
M. Hiza, Acting Chief

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

Thermophysics Division
H. Raveche, Chief

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

Chemical Process Metrology Division
J. Ulbrecht, Chief

- Fluid Flow
  (P. Purtell)
- Multiphase Reacting Flows
  (G. Kulin, Acting)
- High Temperature Reacting Flows
  (H. Semerjian)
- Process Sensing
  (J. Whetstone)

* Located in Boulder

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@R. Hardin
@G. Maloney
N. Sanchez
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@K. Timmerhaus

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@K. Niiya
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*R. Puentes
@D. Reed
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J. Siegwarth
C. Sindt
W. Steward
*S. Valverde
I. Vazquez
R. Voth
J. Way

Properties of Fluids
H. Hanley, Group Leader

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D. Diller
#B. Eaton
J. Ely
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D. Friend
R. Goodwin
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@J. Kuhach
@S. Leffler
#J. Magee
J. Mayrath
R. McCarty
**R. Miller
@Y. Oshmyansky
**M. Paulaitis
J. Rainwater
H. Roder
§K. Romig
**E. Sloan
G. Straty
L. Weber
F. Williamson
B. Younglove

Properties of Solids
L. Sparks, Group Leader

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B. Filla
J. Hurley
J. Hust
R. Radebaugh
**D. Smith
S. Sullivan

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C. Pelanne
A. DiSalvo

*COOP - Cooperative Student Program
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***Part Time
@Intermittent
#National Research Council Postdoctoral Fellow
§National Engineering Laboratory Fellow
†1-Year Detail to Program Office

Thermophysics Division (774)
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C. Thomas, Secretary
K. Hellers, Secretary
L. Phillips, Clerk-Typist

Division Programs

Thermodynamic Modeling - J. Gallagher
L. Haar
**J. Kestin

Condensed Matter - R. Mountain (Leader)
P. Basu (Guest Worker)

Interfacial Phenomena - M. Moldover (Leader)
J. Schmidt
*H. Chaar
T. Edwards (Guest Worker)
J. Rasaiah (Guest Worker)
J. Trusler (Guest Worker)
#R. Berg

Dynamic Measurements - A. Cezairliyan (Leader)
A. Miller

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J. McClure

Statistical Physics
J. Kincaid, Group Leader

**J. Dorfman
J. Hubbard
R. Kayser
***R. MacDonald
@F. Martinez
L. Schmid
@J. Sengers
D. Tsai
D. Jonah (Guest Worker)
M. Klein (Guest Worker)
S. Lee (Guest Worker)
O. Manley (Guest Worker)

Equation of State
J. Levelt Sengers, Group Leader

R. Chang
H. Davis
§M. Emeruwa
§C. Everhart
@J. Manley
G. Morrison
#G. Nielson
K. Johnson (Guest Worker)
D. Linsky (Guest Worker)
B. Taggart (Guest Worker)
H. Woolley (Guest Worker)
§D. Stillo

*COOP - Cooperative Student Program
**University Faculty Appointment (Intermittent)
***Part Time
@Intermittent
#National Research Council Postdoctoral Fellow
§National Engineering Laboratory Fellow

Chemical Process Metrology Division (775)
J. Ulbrecht, Chief
S. Johnson, Secretary
P. Magruder, Secretary
C. Mueller, Secretary

Fluid Flow
P. Purtell, Act. Group Leader

G. Baumgarten
K. Benson
W. Cleveland
**C. Crowe
R. Davis
J. Hall
G. Mattingly
N. Mease
E. Rodriguez
M. Ashmawey (Guest Worker)
W. Rowland (Guest Worker)
K. Tidstrom (Guest Worker)
G. Schubauer (Guest Worker)

Multiphase Reacting Flows
G. Kulin, Act. Group Leader

A. Gaigalas
J. Houser
**D. Loebbaka
K. Lofquist
***E. Moore
B. Robertson
T. Yeh
§N. Bryner
R. Calabrese (Guest Worker)
K. Yuk (Guest Worker)
A. Ghosh (Guest Worker)

High Temperature Reacting Flow
H. Semerjian, Group Leader

J. Allen
*N. Amin
*J. Baumann
R. Charagundla
@P. David
M. Glover
#J. Horvath
A. Macek
C. Presser
#R. Preston
S. Ray
R. Santoro
@D. Shaw
B. Shomaker

Process Sensing
J. Whetstone, Group Leader

@M. Carrier
#D. Cox
@T. Dietz
S. Hasegawa
P. Huang
F. Jones
K. Kreider
J. Melvin
J. Potzick
G. Scace
S. Semancik
@S. Woo

*COOP - Cooperative Student Program
**University Faculty Appointment (Intermittent)
***Part Time
@Intermittent
#National Research Council Postdoctoral Fellow
§National Engineering Laboratory Fellow

Services Contracted
P. Klebanoff
E. James Davis
A. Gupta

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.

CENTER FOR MATERIALS SCIENCE: 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 in the measurement, theory, and prediction of the thermophysical properties of fluids and solid materials of importance to the chemical process industries; performs basic and applied research in unit operations (such as heat and mass transfer, separation, and mixing), systems engineering, thermodynamic analysis of industrial subprocesses, and scale-up; and 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 under equilibrium and nonequilibrium conditions, e.g., multicomponent-multiphase fluid mixtures, interfacial phase transitions, nucleation, critical-point phenomena, phase separation, and transport processes in fluids and high-melting temperature metals; and in close coordination with the Chemical Engineering Science Division, provides critically evaluated technical information (data, theoretical models, computer models) on these thermophysical properties.

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)

Neil A. Olien, Chief

(Fiscal Year 1984)

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 tasks, and with the Chemical Process Metrology Division in flow research. These collaborations include several joint projects sponsored by other agencies, and new ones are currently being pursued.

One of the primary focuses of the 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, such as with the highly accurate measurement and modeling of properties of ethylene and water and the lower molar mass alkanes. The majority of the effort, however, is directed toward problems of the future. These include, but are not restricted to, the following: 1) fluids and processes encountered in the conversion of coal to synthesis gas, methanol, etc., for use as chemical feedstocks; 2) fluids, materials, and processes encountered in the conversion of coal and oil shale to liquid and gaseous fuels which, in turn, contain substantial amounts of aromatic organics and associating (N,O,S) compounds; 3) biomass derivatives as fuel and chemical feedstocks, e.g. alcohol systems; 4) the efficient use of heavy oils, tar sands, and other highly viscous fluids which exhibit nearly solid-like behavior; and 5) the utilization of less energy intensive separation processes. The strategy is to perform basic research, generic to the science underlying the chemical processing and petrochemical 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 separations research has been expanded somewhat, and it is planned to further increase separations research as appropriate new tasks are identified and new funding is secured. The stirred tank mixing research, on the other hand, has reached a logical stopping point, and this marginally-funded effort will be temporarily suspended until resources become available to adequately address the associated issues. The main goals of the transient heat transfer project have been met and this work will be redirected in the forthcoming year. New research on thermal properties of ceramics and polymer composites appears attractive and plans are being developed to identify an appropriate role for the Division.

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 reliable reference data; standard measurement procedures and test methods; predictive techniques, correlations, computer codes, and underlying theory needed by the chemical process industry (CPI) 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 in order to develop new measurement techniques and provide 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 the above efforts will be 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.

° Unit Operations/Processes - M.J. Hiza, Group Leader

The Unit Operations Group performs experimental, theoretical, and mathematical modeling research in: mass transfer, including separations, liquid membranes, and chemical complexation; heat transfer; mixing, including the development of performance standards for stirred tank mixers; flow measurement, including facilities for mass-based gas and cryogenic liquid flow; and process thermodynamics, the analysis of processes and techniques. The composition of the group staff is:

19 full time permanent professionals
2 full time permanent technicians
1 full time permanent secretary
2 part time professionals
4 COOP students
3 intermittent university faculty appointments, (all chemical engineers)
3 students
1 industrial research associate

° 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. Our output is 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, etc. The composition of the group staff is:

- 15 full time permanent professionals
- 1 full time secretary
- 2 National Research Council postdoctoral fellows
- 2 part time professionals
- 3 graduate students (2 Ph.D.'s, 1 MS)
- 1 COOP student
- 3 intermittent university faculty appointments (all chemical engineers)
- 5 guest workers, faculty
- 4 students

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

The research of the Solid Properties Group is focused primarily on experimental and correlative work in the areas of: solid fuels (thermal properties and *SRM's for coal, oil shale, and gas hydrates) and other geological materials; SRM's for fibrous insulation standards; thermal conductivity, thermal expansion, heat capacity, and coefficient of friction of foam, fiber, fiberboard, insulating concretes, aggregates, metals, and polymers; thermal properties of solids for regenerative type refrigerators; and ignition and combustion characteristics of selected metals in oxygen at pressures up to 40 MPa. The composition of the group staff is:

- 8 full time permanent professionals
- 1 full time permanent secretary
- 1 intermittent university faculty appointment

*Standard Reference Materials

4. SELECTED PROJECT SUMMARIES

UNIT OPERATIONS/PROCESSES GROUP

Separations Research - Measurements, Standards, and Modeling

R.D. Noble, J.D. Way, A.L. Bunge, G.J. Hanna, and K.M. Larson

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, azeotropic distillation, and others. Measurement will be for basic transport properties and mass tranfer data, and the resulting fundamental models can 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 and CO_2 removal from gas streams, and removal of metal ions such as copper and organics such as amines from aqueous streams. A new thrust in biotechnology has been initiated. Extraction of acetic and citric acid from aqueous solutions, using both emulsion and immobilized liquid membranes, has been studied. Modeling efforts are tied closely to the experimental program. Models to predict organics removal from aqueous solutions with emulsion liquid membranes, effects of competitive reactions on facilitated transport, and effects of charged species on facilitated transport have been developed. 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. Dr. Subhas K. Sikdar, a chemical engineer with General Electric Corporate Research Laboratories in Schenectady, New York spent one year in our laboratory. He conducted research on the separation of carboxylic acids using ion-exchange membranes.

Mixing Research - Measurement Tests and Standards

R.O. Voth, D.M. Ginley, S. Valverde, and S-J. Khang

The emphasis of this project has been to develop standard performance tests and measurement techniques for stirred tank mixers for a range of fluid and fluid-solid systems. Stirred tank mixers are used throughout the chemical process industry for a wide variety of reasons; consequently, the number of problem areas can be quite diverse. The efforts of this program are directed toward standard tests and measurement methods which will have the most general impact and improvement on mixing operations.

Bench-scale tests have been performed with container sizes of approximately 20 liters or less, to determine mixing rates as a function of time and power input for the dissolution of a solid electrolyte in distilled water. Intrusive conductance probes are used as the detectors; an automated feed tube is used to introduce a known amount of solid into the mixing chamber in a repeatable manner. The experimental control and data acquisition are done with a microcomputer. Experimental results to date, will be documented in an NBS Report.

A five-year research plan was developed and included larger scale test facilities with capacities of 1200-3000 liters. However, the decision was made in the latter part of the year to temporarily suspend this mixing project at the end of FY84, document results achieved, and divert the resources into higher priority research areas. We expect that the work will be reinstated sometime in the future.

Transient Heat Transfer

V.D. Arp, P.J. Giarratano, J.M. Persichetti, W.G. Steward, and D.L. Archuleta

The objective of this research program is to gain a fundamental understanding of the mechanisms of heat transfer in the time domain of one second or less, particularly that involved in large magnitude, short duration heat pulses. The quasi steady-state correlations currently used to model transient heat transfer are known to be incorrect and can result in substantial inaccuracies in predicting behavior in a variety of applications ranging from fission reactors to direct contact heat exchangers. The NBS work combines theoretical studies with two types of experimental measurements. One experimental study, essentially completed, 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 uses 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. The near zero-gravity experiments eliminate the substantial effects of buoyancy. The results will be incorporated into advanced computer codes. The optical facility is useable for a variety of heat and mass transfer studies.

Metering of Natural Gas and Cryogenic Liquids

D.B. Mann, B.R. Bateman, J.A. Brennan, S.E. McManus, C.F. Sindt, and J.D. Siegwarth

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. The 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 flow conditioning concepts and required straight pipe lengths. The work in Boulder using nitrogen gas flow is closely coordinated with similar work on water test fluid in Division 775 (sponsored by the American Petroleum Institute). Both Divisions are participating in a set of field tests at Joliet, Illinois, with pipeline natural gas. The second area of flow research utilizes the flow facility to conduct flow research (e.g. using turbine flowmeters) and perform special tests on meters providing industrial measurement traceability. These tests are performed with liquid nitrogen. The third area of flow research is concerned with high velocity flows (over 50 m/s), and utilize water from a hydro-plant since such velocities are well beyond the range available in a laboratory. The purpose of the work is to assist NASA in developing reliable and safe flowmeters for the Space Shuttle Propulsion system. The last area of research is aimed at providing a liquefied natural gas (LNG) measurements manual which will cover all aspects of custody transfer including flow measurements. This latter project is supported by an international consortium of gas importing firms.

Process Thermodynamics

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

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

PROPERTIES OF FLUIDS GROUP

Integrated Study of Fluid Properties

H.J.M. Hanley, Group Leader

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, 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 coordinate the experimental and theoretical studies. Fluids are selected to be of interest for themselves, but which can be taken as typical of a wide class of industrially important systems. For example, hydrogen sulfide, carbon dioxide, and carbon monoxide are relevant for themselves as components of syngas 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 interest in themselves (such as in the problem of supercritical extraction) but are further typical of industrially important mixtures which invariably contain components of differing chemical nature, size and/or polarity. An important final objective is to develop predictive procedures packaged in the most appropriate form for the user. This work is the core of the fluid property program and is funded jointly by Department of Energy (DOE)-Office of Basic Energy Sciences, Gas Research Institute (GRI)-Basic Research, and the NBS-Office of Standard Reference Data.

Supercritical Fluid Properties

J.F. Ely, J.R. Fox, W.M. Haynes, and L.A. Weber

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. This project, which is supported by a consortium of 14 companies and industrial trade organizations, is developing accurate predictive models for this type of fluid as well as a base of accurate experimental data which can be used to test and further develop the predictive models.

Thus far, this project has produced: 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; and experimental data on selected carbon dioxide/nitrogen systems. Current work emphasizes experimental phase equilibrium measurements on the ternary system carbon dioxide/n-butane/R13 in the temperature range 0 - 200°C with pressures to 30 MPa. In addition, work has been initiated to develop wide range equations of state for various halohydrocarbons which are of interest in supercritical fluid extraction.

Viscosity and Thermal Conductivity Measurements

D.E. Diller and H.M. Roder

Measurements on viscosity and thermal conductivity are vital to complete the data 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 the academic standpoint and demonstrates the fascinating and versatile behavior of a fluid in nonequilibrium. We have an ongoing program to measure the viscosities of liquids and mixtures from 80-320 K from the gas to the very dense liquid 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. The latest results are for methane/ethane mixtures and, among other highlights, show most unusual and currently not understood critical region behavior. A new viscometer has been built which can operate at temperatures to 600 K. This apparatus will undergo testing shortly. Systems for study will be the "C_6 compounds" -- benzene, cyclohexane, and hexane.

Properties of Chemically Reacting Systems

J.E. Mayrath, T.J. Bruno, and H.J.M. Hanley

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 proposed a philosophical guideline suggesting steps that the experimentalist 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 what we consider the minimum equipment needed to analyze the composition of possible reacting fluids. The equipment consists of a gas chromatograph, liquid chromatograph, ultraviolet spectrophotometer, and an infrared spectrophotometer. The whole laboratory is explosion proof and can handle toxic substances. We have already experienced the problems of reactive test fluids with our PVT measurements of H_2S and methanol 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 with our supercritical gas chromatograph.

Phase Equilibria Data for Industrial Fluids

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

Phase equilibria (VLE, LLE, 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 300-450 K. The systems CO_2/n-butane, CO_2/i-butane are being studied. The object is to better understand the influence of the isomers in an organic/inorganic mixture; CO_2/halogenated hydrocarbons are planned for further work. A high temperature VLE apparatus for operation from 300-900 K is available and being refined. 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 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/sec) 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 and 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. 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/C_1 mixtures and H_2/C_3 mixtures. H_2/CO_2 studies are in progress. Finally we plan to use the magnetic densimeter to investigate LLE of cryogenic mixtures: the results are of interest to support our corresponding states predictions.

PVT Measurements of Industrial Fluids

G.C. Straty and W.M. Haynes

The group has three operational apparatuses to measure the PVT properties of fluids: a direct density measurement magnetic densimeter operating between 80 and 320 K for pressures to 35 MPa, a 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, and methanol.

Prediction of Fluid Properties

R.D. McCarty, R.D. Goodwin, J.F. Ely, D.G. Friend, J.C. Rainwater, and 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 in science or engineering. Correlations for several pure fluids have been published recently: H_2S, CO, CO_2, ethylene, for example. Prediction packages include TRAPP (transport property prediction procedure), FLUID PACK (properties of pure fluids) and SUPERTRAP (phase equilibria, properties of mixtures) to be released soon. These procedures are the visible result 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.

Fundamentals of Fluid Behavior: Equilibrium and Nonequilibrium

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

A long-term investigation is underway to study the behavior 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, i.e., 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 out of 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.

Measurement of Thermodynamic Properties of Fluids

J.W. Magee and B.A. Younglove

There is an awareness in industry that data for the derived, or thermodynamic properties (e.g., specific heat, velocity of sound, enthalpy, etc.) 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. We are measuring the specific heat of CO_2, the specific heat of methane/ethane mixtures, and the velocity of sound of natural gas type mixtures. All these results are of immediate relevance to the gas industry. We also need them to develop our theoretically based prediction procedures.

Association in Coal Liquids

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

Predictive procedures that are, in general, successful for relatively simple mixtures can fail when they are 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 a parameter to enter into the appropriate prediction procedure. We are evaluating straightforward measurements of a) heats of mixing and b) viscosity to determine if they will provide this information. We construct model coal liquids with known associating compounds for these quantitative investigations.

PROPERTIES OF SOLIDS GROUP

Solid Fuels Research

J.E. Callanan and S.A. Sullivan

During the development of transferable measurement techniques for the specific heat capacity of coal and char, an evolution of water from supposedly dried coals was observed. The Merrick model, as activated by R. MacDonald of Division 774, was modified to allow evolution of gases below 573 K. The model confirms that only water is evolved in this temperature range as well as the temperatures at which this evolution is observed. The model only partially accounts for the observed dependence of the heat capacity on the gaseous atmosphere present in the specimen cells. Collaborative studies made on our specimens at Sandia National Laboratory (Livermore) corroborate the evidence from both experiment and modeling.

Delivery of coal macerals from Southern Illinois University and the first premium coal from Argonne National Laboratory are now overdue. The transferable measurement techniques will be applied to these specimens. Heat capacity as a function of rank will be evaluated for a rank-series of coals which have been studied at SIU by photoacoustic techniques.

Funding has been received from DoE, Morgantown in partial support of the work on gas hydrates. A hydrate preparation chamber has been built and a cutting device for producing samples has been designed. The thermal expansion apparatus has been recalibrated to provide greater sensitivity for the measurements. The model development by R. Mountain, Division 774, is proceeding in collaboration with M. Klein of the National Research Council of Canada (Ottawa).

Further calibration of the DSC with high-pressure cells, particularly in the sub-ambient region, is required both for heat capacity measurement of hydrates and for studies of coal at higher temperatures.

The hot-wire thermal conductivity apparatus is complete except for testing the logic related to the scanner and construction of the retort and required specimen holders. Upon delivery of the scanner this work will be completed and, after testing on known materials, thermal conductivity measurements of coals can be initiated.

An exploratory study of the measurement of elastic constants and internal friction of coal by oscillator and resonance techniques has been successful. Voids (pores) and changes in voids can be studied with these techniques; this will allow the evaluation of effects of various heating regimes on the thermal properties of coal. This study was performed in collaboration with the NBS Fracture and Deformation Division in Boulder, Colorado.

Materials for LNG Applications: Insulating Foams and Concretes

L.L. Sparks

Properties of several materials which are used in the transport and storage of liquefied fuels were studied. Two basic types of material are of particular interest: insulating foams and insulating concretes. Because of unique structural/insulating capabilities, these materials are being widely used in industry in spite of an extremely uncertain data base. Both materials are being experimentally studied in the temperature range from near 76 K to 350 K. The properties of interest are thermal conductivity, thermal expansion, and tensile, compressive, and shear strengths and their moduli. In the case of the expanded plastic foams, polyurethane is the material being studied. The experimental data and characterization of the cell morphology are used in analytical models for low temperature behavior. Insulating, or lightweight, concretes are not at the same level of development as the foams. Data were generated for portland cement/polystyrene, portland cement/vermiculite, and polyester/lightweight aggregate in order to identify a type of material combination for further study. This work is performed in cooperation with the NBS Fracture and Deformation Division in Boulder, Colorado.

Development of SRM's and SRD

J.G. Hust, D.R. Smith, A.B. Lankford, J.E. Callanan, and S.A. Sullivan

Research has been directed toward the establishment and extension of several thermal property Standard Reference Materials (SRM's) and toward the establishment of Standard Reference Data (SRD) for several metals. Thermal conductivity standard reference data have been published for aluminum, copper, iron, and tungsten from liquid helium temperature to the melting point of each metal. These data are presented in the form of graphs, tables, and equations as a function of temperature and electrical residual resistivity.

A "lot" of fine-grained graphite has been established as an SRM for thermal conductivity and electrical resistivity. This SRM is the result of a world-wide cooperative program that started in 1977 and encompasses several existing SRM's and several thermophysical properties. Certification of this lot of graphite for other properties is anticipated on the basis of this wide-ranging measurement effort.

Research has continued to extend the certification of a glass fiberboard thermal conductance SRM to temperatures below 255 K. In addition, a glass fiberblanket material is being certified as a thermal conductance SRM at temperatures from 100 to 330 K. A high-temperature guarded-hot-plate apparatus is being constructed for use in establishing similar insulation SRM's at temperatures up to 800 K. The high temperature program is closely coordinated with the efforts of the insulation industry.

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

A study of the feasibility of developing temperature and enthalpy of fusion standards for differential scanning calorimetry with the differential scanning calorimeter (DSC) has shown that this can be done successfully. Four standards have been developed in FY 84 as part of a long-range effort in the development of temperature and enthalpy of fusion standards. A proposal for a feasibility study for standards development for heat capacity using the DSC has been funded for FY 85.

Cryocooler Studies

R. Radebaugh, B. Louie, and D.R. Smith

Most of the inefficiency in regenerative refrigerators operating below about 20 K is due to the regenerator ineffectiveness. A program funded by the David Taylor Naval Ship R and D Center and the Office of Naval Research has led to a simple design technique which gives the optimum geometry parameters for regenerators. The technique is being expanded to include various non-ideal conditions. The design technique was just presented at the Third Cryocooler Conference, September 17-18, 1984, held at NBS Boulder under the chairmanship of R. Radebaugh.

Under a five-year Air Force contract, a regenerator test apparatus has been built and measurements of thermal properties of lead powder have been made. Measurements of new materials and new geometries will be made over the next five years under a new Air Force contract to greatly improve these low temperature regenerators. A computer model has been developed and will be checked against the forthcoming experimental results on new materials and geometries.

A new type of refrigeration, known as pulse tube or thermoacoustic refrigeration, has the potential for high reliability because there are no moving parts at low temperature. The intrinsic behavior of three different modes of thermoacoustic refrigeration are being studied under a NASA/Ames contract. Transient heat transfer is important in this refrigeration method, particularly at the higher frequencies near 1 kHz. A demonstration refrigerator to reach temperatures below 100 K will be built for NASA.

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 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). Emission spectra and high-speed movies are also obtained.

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.

Low-Temperature Properties of Cryogenic Refrigerator Sealing Materials

L.L. Sparks

Reliable, long-life cryogenic cooling is essential to the development and operation of space-based infrared surveillance systems. The Vuilleumier cycle cryocooler has unique advantages for systems that must be capable of long, unattended operation. The goal for this Air Force system is five years of orbital service. The low-temperature properties of the dynamic seals and riders are essential. NBS is working in cooperation with Air Force Wright Aeronautical Laboratory and Hughes Aircraft Company to develop and evaluate candidate materials. Reinforced resin composites are currently being developed and wear tested at Hughes, while the basic properties of thermal contraction, coefficient of friction, and tensile and shear properties are being studied at NBS. The temperature range of study is from 10 to 300 K. This work is performed cooperatively with the Fracture and Deformation Division in Boulder, Colorado.

5. HONORS AND AWARDS

James A. Brennan - American Gas Association Operating Section Award of Merit for his work and contributions as a member of the Transmission Measurements Committee.

Patricia J. Giarratano - Department of Commerce, Bronze Medal Award for her work on transient heat transfer between solid and fluid phases in near zero gravity.

Howard J.M. Hanley - Chairman-elect of 9th Symposium on Thermophysical Properties (1985), co-sponsored by the ASME and International Thermophysics Congress.

- Guest Editor, Physics Today (January 1984).

Elaine G. Hunnel - Department of Commerce, Bronze Medal Award for her novel contributions to administrative procedures, resulting in peak efficacy in management of government resources.

6. PUBLICATIONS

Published

Arp, V.D., Daney, D.E., Giarratano, P.J., and Steward, W.G., Transient heat transfer processes, AIChE Symp. Series, Vol. 79, No. 224, pp. 126-132 (1983).

Arp, V.D., Persichetti, J.M. and Guo-Bang, C., The Gruneisen parameter in fluids, J. of Fluids Eng., Vol. 106, pp. 193-201 (June 1984).

Bateman, B.R., Way, J.D. and Larson, K.M., An apparatus for the measurement of gas fluxes through immobilized liquid membranes, Sep. Sci. Tech., Vol. 19, No. 1, pp. 21-32 (1984).

Bransford, J.W., High pressure polycrystalline sodium chloride window and mounting arrangement for CO_2 laser transmission, Rev. Sci. Instrum., Vol. 55, No. 1, pp. 125-126 (Jan. 1984).

Bruno, T.J., Instrumental aspects of supercritical fluid chromatography, Proc. of the 2nd Sym. on Energy Eng. Sci., Argonne Nat. Lab., Argonne, IL, pp. 78-85 (1984).

Daney, D.E. and Radebaugh, R., Non-ideal regenerator performance--the effect of void volume fluid heat capacity, Cryogenics, Vol. 24, No. 9, pp. 499-501 (Sept. 1984).

Diller, D.E., Development of a high temperature (600 K), high pressure (100 MPa) viscometer, Proc. of the 2nd Sym. on Energy Eng. Sci., Argonne Nat. Lab., Argonne, IL, pp. 49-53 (1984).

Diller, D.E., Measurements of the viscosity of compressed gaseous and liquid methane + ethane mixtures, J. Chem. Eng. Data, Vol. 29, No. 2, pp. 215-221 (April 1984).

Diller, D.E., Shear viscosity coefficients of nitrogen + methane and methane + ethane mixtures, The Am. Soc. Mech. Eng., Pap. No. 83-WA/HT-49, 1983 Winter Annual Meeting, Boston, MA (Nov. 14-18, 1983).

Ely, J.F., Application of the extended corresponding states model to hydrocarbon mixtures (Computer Program EXCST), Proc. of the 63rd Annual Convention, Gas Processors Assoc., Tulsa, OK, pp. 9-22 (1984).

Ely, J.F. and Baker, J.K., A review of supercritical fluid extraction, Nat. Bur. Stand. (U.S.) Tech. Note 1070 (Dec. 1983).

Evans, D.J., Hanley, H.J.M., and Hess, S., Non-Newtonian phenomena in simple fluids, Phys. Today, Vol. 37, No. 1, pp. 26-33 (1984).

Flynn, T.M., Cryogenic processes, Perry's Chem. Eng. Handbook, Subsection of Sec. 12, pp. 12-47 and 12-58, 6th Edition (McGraw-Hill, NY 1984).

Fox, J.R., Method construction of nonclassical equations of state, Fluid Phase Equilibria, Vol. 14, pp. 45-53 (1983).

Friend, D.G., The radial distribution function at low densities: Exact results for small and large separations for smooth potentials, J. Chem. Phys., Vol. 79, No. 9, p. 4553 (Nov. 1983).

Friend, D.G. and Rainwater, J.C., Transport properties of a moderately dense gas, Chem. Phys. Lett., Vol. 107, No. 6, pp. 590-594 (June 1984).

Giarratano, P.J., Transient boiling heat transfer from two different heat sources: Small diameter wire and thin film flat surface on a quartz substrate, Int. J. Heat Mass Trans., Vol. 27, No. 8, pp. 1311-1318 (1984).

Goodwin, R.D., Carbon monoxide compressibility data from 100 to 300 K, derived virial coefficients, orthobaric densities and heats of vaporization, Cryog., Vol. 23, No. 8, pp. 403-414 (Aug. 1983).

Goodwin, R.D., Hydrogen sulfide provisional thermophysical properties from 188 to 700 K at pressures to 75 MPa, Nat. Bur. Stand. (U.S.) Interim Report 83-1694 (Oct. 1983).

Hanley, H.J.M., Thermophysical properties of fluids for the gas industry, Gas Res. Inst., Annual Report, GRI-84/0042, 37 pp (1984).

Hanley, H.J.M., Prediction of transport properties: Application of basic theory, Rev. of Portugese Chemistry, Vol. 25, pp. 27-35 (1983).

Hanley, H.J.M., Rainwater, J.C., Clark, N.A. and Ackerson, B.J., Liquid structure under shear: Comparison between computer simulations and colloidal suspensions, J. Chem. Phys., Vol. 79, No. 9, pp. 4448-4458 (Nov. 1983).

Haynes, W.M., Orthobaric liquid densities and dielectric constants of (methane + 2-methyl-propane) and (methane + butane) at low temperatures, J. Chem. Thermodyn., Vol. 15, pp. 903-911 (1983).

Haynes, W.M., Kidnay, A.J., Olien, N.A. and Hiza, M.J., Status of thermophysical properties data for pure fluids and mixtures of cryogenic interest, Adv. Cryog. Eng., Vol. 27, pp. 919-942 (1984).

Haynes, W.M., McCarty, R.D. and Hiza, M.J., Liquefied natural gas densities: Summary of research program at the NBS, Nat. Bur. Stand. (U.S.) Monograph 172 (Oct. 1983).

Hess, S. and Hanley, H.J.M., The pressure tensor and viscosity coefficients of a soft sphere liquid under shear, Int. J. Thermophys., Vol. 4, No. 2, pp. 97-114 (1983).

Hess, S. and Hanley, H.J.M., Stokes-Maxwell relations for the distorted fluid microstructure, Phys. Lett., Vol. 98A, No. 1,2, pp. 35-38 (Oct. 1983).

Hess, S., Hanley, H.J.M. and Herdegen, N., Nonlinear flow behavior of gases, Phys. Lett., Vol. 105A, No. 4,5, pp. 238-240 (Oct. 15, 1984).

Hess, S. and Rainwater, J.C., Diffusion in a laminar flow: Shear rate dependence of correlation functions and of effective transport coefficients, J. Chem. Phys., Vol. 80, No. 3, pp. 1295-1303 (Feb. 1984).

Holland, P.M., Eaton, B.E., and Hanley, H.J.M., A correlation of the viscosity and thermal conductivity data of gaseous and liquid ethylene, J. Phys. Chem. Ref. Data, Vol. 12, No. 4, pp. 917-932 (1983).

Hord, J., Snapshot of the NBS Center for Chemical Engineering, National Conf. of Standards Laboratories, 1983 Workshop and Symposium, I-3.1 thru I.3-9 (Hilton Harvest House, Boulder, CO, 1983).

Hust, J.G., Thermal conductivity of glass fiber/epoxy composite support bands for cryogenic dewars, phase II, Nat. Bur. Stand. (U.S.) Interim Report 84-3003 (March 1984).

Hust, J.G., A fine-grained, isotropic graphite for use as NBS thermophysical property SRM's from 5 to 2500 K, Nat. Bur. Stand. (U.S.) Spec. Pub. 260-89 (Sept. 1984).

Hust, J.G. and Lankford, A.B., Thermal conductivity of aluminum, copper, iron, and tungsten for temperatures from 1K to the melting point, Nat. Bur. of Stand. (U.S.) Interim Report 84-3007 (June 1984).

Hust, J.G. and Lankford, A.B., Update of thermal conductivity and electrical resistivity of electrolytic iron, tungsten, and stainless steel, Nat. Bur. Stand. (U.S.) Spec. Pub. 260-90 (Sept. 1984).

Jahangiri, M., Jacobsen, R.T., Stewart, R.B. and McCarty, R.D., Thermodynamic properties of ethylene at saturation, Adv. Cryog. Eng., Vol. 29, pp. 965-972 (Plenum Press, NY, 1984).

Kidnay, A.J., Olien, N.A. and Hiza, M.J., The status of thermophysical properties data for pure fluids and mixtures at low temperatures, AIChE Symp. Ser., Vol. 70, No. 224, pp. 105-113 (1983).

Mann, D.B., Brennan, J.A., Sindt, C.F., LaBrecque, J.F., McManus, S.E. and Kneebone, C.H., Gas orifice meter discharge coefficients as determined by mass flow measurements, Int. Conf. on the Metering of Natural Gas and Liquefied Hydrocarbon Gases, pp.1-20 (London, England, 1984).

Masui, R., Haynes, W.M., Chang, R.F., Davis, H.A. and Sengers, J.M.H.L., Densimetry in compressed fluids by combining hydrostatic weighing and magnetic levitation, Rev. Sci. Instrum., Vol. 55, No. 7, pp. 1132-1142 (July 1984).

Noble, R.D. and Kemp, N.J., Heat transfer effects in facilitated transport liquid membranes, Sep. Sci. Tech., Vol. 18, No. 15, pp. 1147-1165 (1984).

Noble, R.D., Buschman, R.G. and Kemp, N.J., Vertical temperature distribution in lakes, J. Environ. Syst., Vol. 14, No. 1, pp. 63-75 (1984-1985).

Olien, N.A. and Raveche, H.J., Thermophysical property data generated by the NBS Center for Chem. Eng., AIChE Symp. Ser., Vol. 80, No. 237, pp. 101-107 (1984).

Radebaugh, R., Very low temperature cooling systems, Cryocoolers, Part 2: Applications, Chap. 12, pp. 177-255 (Plenum Press, NY 1983).

Radebaugh, R., Fundamentals of alternate cooling systems, Cryocoolers, Part 2: Applications, Chap. 11, pp. 129-175 (Plenum Press, NY 1983).

Rainwater, J.C., On the phase space subdivision of the second virial coefficient and its consequences for kinetic theory, J. Chem. Phys., Vol. 81, No. 1, pp. 495-510 (July 1984).

Roder, H.M., Experimental thermal conductivity measurements on hydrogen, methane, ethane and propane, Nat. Bur. Stand. (U.S.) Interim Report 84-3006 (May 1984).

Siegwarth, J.D., LaBrecque, J.F. and Carroll, C.L., Volume uncertainty of a large tank calibrated by photogrammetry, A volume uncertainty of 0.03 percent was obtained, Photogramm. Eng. and Remote Sensing, Vol. 50, No. 8, pp. 1127-1134 (Aug. 1984).

Sparks, L.L. and Arvidson, J.M., Thermal and mechanical properties of polyurethane foams and a survey of insulating concretes at cryogenic temperatures, Gas Res. Inst., Final Report GRI 84/0086, Jan. 1979-Feb. 1984 (April 1984).

Wankat, P.C. and Noble, R.D., Calculations for separations with three phases. 2. Continuous contact systems, Ind. Eng. Chem. Fundam., Vol. 23, No. 2, pp. 137-143 (1984).

Weber, L.A., Apparatus for moderate temperature VLE measurements of CO_2-isobutane systems, Proc. of the 2nd Sym. on Energy Eng. Sci., Argonne Nat. Lab., Argonne, IL, pp. 10-16 (1984).

Publications in Progress

Bransford, J.W., Laser-initiated combustion studies on metallic alloys in pressurized oxygen, Nat. Bur. Stand. (U.S.) Interim Report.

Bransford, J.W., Ignition of metals in high pressure oxygen, in Conf. Proceedings: Advanced High Pressure O_2/H_2 Tech. Conf.

Callanan, J.E. and Filla, B.J., A laboratory-scale controlled-atmosphere chamber for use with premium coal samples, Rev. Sci. Instrum.

Diller, D.E. and Van Poolen, L.J., Tests of models for the shear viscosity coefficients of compressed and liquefied hydrocarbon gases, J. High Temp. High Pressure.

Diller, D.E. and VanPoolen, L.J., Measurements of the viscosities of saturated and compressed liquid normal butane and isobutane, Int. J. Thermophys.

Friend, D.G., The phase space subdivision of the second virial coefficient, J. Chem. Phys.

Goodwin, R.D., Benzene thermophysical properties from 279 to 900K at pressures to 100 MPa, J. Phys. Chem. Ref. Data.

Hanna, G.J. and Larson, K.M., The influence of preparation parameters on internal droplet size distribution of emulsion liquid membranes, Ind. Eng. Chem. Prod. Res. Dev.

Haynes, W.M., Orthobaric liquid densities and dielectric constants of ethylene, Cryogenics.

Haynes, W.M., McCarty, R.D., Eaton, B.E. and Holste, J.C., Isochoric (p,V,T) measurements on (methane + ethane) from 100 to 320 K at presssures to 35 MPa, J. Chem. Thermodyn.

Kidnay, A.J., Miller, R.C., Sloan, E.D. and Hiza, M.J., A review and evaluation of the phase equilibria, liquid phase heats of mixing and excess volumes, and gas phase PVT measurements for nitrogen + methane, J. Phys. & Chem. Ref. Data.

Louie, B. and Radebaugh, R., The Stirling Cycle and cryogenic refrigerator, Conf. Proc. of the 19th Intersoc. Energy Conversion Eng. Conf., San Francisco, CA, Aug. 19-24, 1984.

Mansoori, G.A. and Ely, J.F., Density expansion (DEX) mixing rules (Thermodynamic modeling of supercritical extraction), J. Chem. Phys.

Mansoori, G.A. and Ely, J.F., Statistical mechanical theory of local compositions, Fluid Phase Equilibria.

Nguyen, K., Bransford, J.W. and Branch, M.C., Ignition phenomena of bulk aluminum alloy as a function of oxygen pressure, Proc. of 21st JANNAF Combustion Meeting.

Niiya, K.Y. and Noble, R.D., Competitive facilitated transport through liquid membranes, J. Membr. Sci.

Noble, R.D., Kinetic efficiency factors for facilitated transport membranes, Chem. Eng. Sci. J.

Roder, H.M., The thermal conductivity of hydrogen, Int. J. Thermophys.

Roder, H.M., The thermal conductivity of methane for temperatures between 110 and 310 K with pressures to 70 MPa, Int. J. Thermophys.

Roder, H.M. and Nietro de Castro, C.A., The thermal conductivity of ethane for temperatures between 110 and 325K with pressures to 70 MPa, Proc. of the 9th European Conf. on Thermophys. Prop.

Siegwarth, J.D., Vortex shedding flowmeters for liquids at high velocities, NASA Conf., Univ. of Alabama, Huntsville, AL (June 27-29, 1984).

Smith, D.R., Hust, J.G. and Van Poolen, L.J., A guarded hot plate apparatus for effective thermal conductivity of insulations at 80-360K, 18th Int. Therm. Conductivity Conf.

Sparks, L.L. and Arvidson, J.M., Thermal and mechanical properties of polyurethane foams at low temperatures, Proc. of the 28th Annual Polyurethane Div. Tech./Marketing Conf.

Straty, G.C., Automated high temperature PVT apparatus with data for propane, Nat. Bur., Stand. (U.S.) J. Res.

Way, J.D., Noble, R.D. and Bateman, B.R., Selection of supports for immobilized liquid membranes, ACS Symp. Series on Membr. Mater. Sci.

Weber, L.A., Vapor-liquid equilibria measurements for carbon dioxide with normal and isobutane from 250 to 280 K, Cryogenics.

7. TALKS

Noble, R.D., Summary of Membrane Research at NBS, DOE Membrane Technology Workshop, Austin, TX, Oct. 28, 1983.

Arp, V.D., and Giarratano, P.J., Review of Transient Heat Transfer Research, Chemical Engineering Science Division Colloquium, Boulder, CO, Sept. 30, 1983.

Diller, D.E., Shear Viscosity Coefficients of Nitrogen + Methane and Methane + Ethane Mixtures, ASME Winter Annual Meeting, Boston, MA, Nov. 15, 1983.

Fox, J.R., Chemical Oscillations, Chemical Engineering Science Division Colloquium, Boulder, CO, Dec. 9, 1983.

Bruno, T.J., Experimental Thermodynamics of Molecular Association, Chemical and Petroleum Refining Engineering Department, Colorado School of Mines, Golden, CO, Dec. 13, 1983

Hord, J., Hydrogen Technology for Space Power, Wright Patterson Air Force Base, Dayton, OH, Dec. 20, 1983.

Noble, R.D., Facilitated Transport of Carbon Monoxide Across Liquid Membranes, Argonne National Laboratory, Argonne, IL, Jan. 1, 1984.

Mann, D.B., Gas Orifice Meter Discharge Coefficient as Determined by Mass Flow Measurements, National Engineering Laboratory, London, England, Feb. 2, 1984.

Olien, N.A., Large Scale Computing Applications in the Center for Chemical Engineering, NBS Computing Evaluation Panel, Center for Applied Mathematics, NBS, Gaithersburg, MD, Feb. 13, 1984.

Olien, N.A., Energy Related Research in the NBS-Center for Chemical Engineering, Pittsburgh Energy Technology Center, Pittsburgh, PA, Feb. 14, 1984.

Hanley, H.J.M., Non-Newtonian Behavior of Simple Liquids, University of Erlangen-Nurnberg, Erlangen, West Germany, Mar. 4, 1984.

Noble, R.D., What Chemical Engineers Do in Research, AIChE Student Chapter, Colorado State University, Fort Collins, CO, Mar. 5, 1984.

Olien, N.A., The Prediction of Reference Data for Thermodynamics and Thermochemistry, The Effect of Computers on the Generation and the Use of Technical Data Workshop, NBS, Gaithersburg, MD, Mar. 19, 1984.

Hanley, H.J.M., Nonequilibrium Simulations of Liquid Behavior, Institute Laue-Langevin, Grenoble, France, Mar. 20, 1984.

Sindt, C.F., Current Work on Basic Orifice Metering Project, Gas Research Institute Meeting, Memphis, TN, Mar. 20, 1984.

Diller, D.E., Measurements of Shear Viscosity Coefficients of Fluids for the Gas Industry, GRI Thermophysical Properties Workshop, New Orleans, LA, Mar. 22, 1984.

Siegwarth, J.D., Target Fabrication, LLNL and LASL Fusion Target Fabrication Conference, San Diego, CA, Apr. 6, 1984.

Noble, R.D., Chemical Complexation Research at the National Bureau of Standards, Department of Chemical Engineering and Chemical Technology, Imperial College, London, England, Apr. 6, 1984.

Olien, N.A., Experimental Capacity for Fluid Measurements with the NBS Center for Chemical Engineering, GRI, Houston, TX, Apr. 10, 1984.

Bruno, T.J., Instrumental Aspects of Supercritical Fluid Chromatography, Second Symposium on Energy Engineering Sciences, Argonne National Laboratory, Argonne, IL, Apr. 10, 1984.

Diller, D.E., Development of a High Temperature (600 K) High Pressure (100 MPa) Viscometer, Second Symposium on Energy Engineering Sciences, Argonne National Laboratory, Argonne, IL, Apr. 10, 1984.

Bateman, B.R., Selection of Supports for Immobilized Liquid Membranes, American Chemical Society, St. Louis, MO, Apr. 11, 1984.

Radebaugh, R., Cryocoolers and Thermal Regenerators, Chemical Engineering Science Division Colloquium, Boulder, CO, May 11, 1984.

Noble, R.D., and Way, J.D., Chemical Complexation Research at the U.S. National Bureau of Standards, Italian Nuclear and Alternate Energy Laboratory (ENEA), Rome, Italy, May 15, 1984.

Hord, J., Research Activities of the NBS Center for Chemical Engineering, Dow Chemical, Midland, MI, May 16, 1984.

Way, J.D., and Noble, R.D., Mathematical Modeling of Gas Separations Using Chemical Complexation, ENEA, Rome, Italy, May 16, 1984.

Noble, R.D., and Way, J.D., Experimental Results of Gas Separations Using Chemical Complexation, ENEA, Rome, Italy, May 17, 1984.

Hanna, G.J., The Influence of Preparation Parameters on Internal Droplet Size Distribution of Emulsion Liquid Membranes, AIChE Meeting, Anaheim, CA, May 22, 1984.

Straty, G.C., Experimental Techniques for PVT Measurements at Elevated Temperature, Lisbon Technical University, Lisbon, Portugal, May 25, 1984.

Straty, G.C., Experimental Techniques for PVT Measurements at Elevated Temperature, Coimbra University, Coimbra, Portugal, May 28, 1984.

Sullivan, S.A., Temperature and Energy Calibration of Differential Scanning Calorimeters, Rocky Mountain Chapter of North American Thermal Analysis Society, Boulder, CO, May 22, 1984.

Way, J.D., and Noble, R.D., Chemical Complexation Research at NBS, Honeywell Research Center, Minneapolis, MN, May 30, 1984.

Noble, R.D., Mathematical Modeling of Chemical Separations, Mankato State University, Mankato, MN, May 31, 1984.

Callanan, J.E., Differential Scanning Calorimetry Measurements of Solids, CAN-AM Congress/Joint Canadian Institute of Chemistry/American Institute of Chemistry Meeting, Montreal, Quebec, Canada, Jun. 5, 1984.

Siegwarth, J.D., Tests of Vortex Shedding Flowmeters at High Liquid Flow Velocities, University of Alabama at Huntsville and NASA High Pressure H_2/O_2 Technology Conference, Huntsville, AL, Jun. 12, 1984.

Way, J.D., Acid Gas Separations Using Chemical Complexation in Ion-Exchange Membranes, DOE Advanced Gasification Projects Contractor Meeting, Morgantown, WV, Jun. 25, 1984.

Bransford, J.W., Ignition of Metals in High Pressure Oxygen, Advanced High Pressure O_2/H_2 Technology Conference, NASA, Huntsville, AL, Jun. 27, 1984.

Noble, R.D. and C.A. Koval, An Iron (II) Macrocyclic Complex Which Acts as a Selective Host for Dissolved Carbon Monoxide and Thereby Facilitates the Transport of Gaseous CO Through Liquid Membranes, 23rd International Conference on Coordination Chemistry, University of Colorado, Boulder, CO, Jul. 29, 1984.

Noble, R.D., Solute Consumption in Emulsion Liquid Membranes, Summer School on Modern Applied Mathematics in Chemical Engineering, Bad Honnef, West Germany, Jul. 31, 1984.

Noble, R.D., A Duet on Double Diffusion, Summer School on Modern Applied Mathematics in Chemical Engineering, Bad Honnef, West Germany, Aug. 8, 1984.

Callanan, J.E., Temperature and Enthalpy Standards Development by DSC for DSC, IUPAC Conference on Chemical Thermodynamics and 39th Annual Calorimetry Conference, McMaster University, Hamilton, Ontario, Canada, Aug. 13, 1984.

Noble, R.D., Gas Separation through Liquid Membranes Containing Carriers, Gordon Research Conference on Separations and Purification, New London, NH, Aug. 13, 1984.

Callanan, J.E., Evaluation of the Desorption of Water from Coal Specimens, Heat of Desorption of Water, IUPAC Conference on Chemical Thermodynamics and 39th Annual Calorimetry Conference, McMaster University, Hamilton, Ontario, Canada, Aug. 16, 1984.

Hanna, G.J., and Larson, K.M., Separations at NBS, High School Honors Institute, University of Colorado, Boulder, CO, Aug. 21, 1984.

Louie, B., The Stirling Cycle and Cryogenic Refrigerators, Intersociety Energy Conversion Engineering Conference, San Francisco, CA, Aug. 23, 1984.

Siegwarth, J.D., Tests of Vortex Shedding Flowmeters at High Liquid Flow Velocities, NBS-Industry-Government Vortex Shedding Consortium Meeting, Division 775, NBS, Gaithersburg, MD, Aug. 29, 1984.

Noble, R.D., Separation of Gases Using Chemical Complexation in Liquid Membranes, Stevens Institute of Technology, Hoboken, NJ, Sep. 6, 1984.

Diller, D.E., Shear Viscosity Coefficients of Compressed and Liquefied Butane Isomers, 9th European Conference on Thermophysical Properties, Manchester, England, Sep. 17, 1984.

Bateman, B.R., Measurements of Flow Properties in a High Pressure Gas System Exhibiting Strong Swirl-Apparatus and Techniques, Chemical Engineering Science Division Colloquium, Boulder, CO, Sep. 28, 1984.

Roder, H.M., The Thermal Conductivity of Simple Fluids, Department of Mechanical and Chemical Engineering, University of New Brunswick, Fredericton, New Brunswick, Canada, Oct. 8, 1984.

Arp, V.D., Transient Heat Transfer and Hydrodynamics, Department of Mechanical Engineering, University of Colorado, Boulder, CO, Oct. 11, 1984.

Rainwater, J.C., Density Corrections to Transport Properties for Gases with Realistic Potentials, Division 774 Seminar, NBS, Gaithersburg, MD, Oct. 15, 1984.

Larson, K.M., Internal Droplet-Size Distribution and Mass Transfer in Emulsion Liquid Membranes, New Directions in Separation Technology Conference, Davos, Switzerland, Oct. 16, 1984.

Rainwater, J.C., Density Corrections to Transport Properties for Gases with Realistic Potentials, University of Maryland, College Park, MD, Oct. 16, 1984.

Noble, R.D., Effectiveness Factors for Facilitated Transport Membranes, New Directions in Separations Technology, Engineering Foundation Conference, Davos, Switzerland, Oct. 16, 1984.

Bruno, T.J., Physicochemical Measurements Using Supercritical Fluid Chromatography, Supercritical Fluid Workshop, NBS, Gaithersburg, MD, Oct. 17, 1984.

Rainwater, J.C., Vapor-Liquid Equilibrium of Near-Critical Binary Mixtures: A Modified Leung-Griffiths Model, Division 774 Seminar, NBS, Gaithersburg, MD, Oct. 18, 1984.

Fox, J.R., Rescaling the Classical Equations of State, Supercritical Fluid Workshop, NBS, Gaithersburg, MD, Oct. 18, 1984.

Bruno, T.J., A New Instrument for Direct Fugacity Measurements in Hydrogen Mixtures, Chemistry Department, Georgetown University, Washington, DC, Oct. 19, 1984.

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

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

J.A. Brennan

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

OIML, U.S. National Working Group, PS5/RS15 (Member)

M.J. Hiza

AIChE Cryogenics Committee (Past Chairman)

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

R.D. Noble

Amer. Soc. for Engr'g. Education (ASEE), Chemical Engineering Division (Member)

ASEE 1984 National Conference Program Committee (Chairman)

ASEE Educational Research and Methods Division (Member and Board of Directors)

ASEE Rocky Mountain Section 1984 (Program Chairman)

J.M. Persichetti

Rocky Mountain Chapter AIChE (Co-secretary)

R.O. Voth

Division 773 Hazards Review Committee (Chairman)

J. Hord

AIChE Research Advisory Committee (Member and Chairman of Oversight Subcommittee)

D.E. Diller

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

Amer. Gas Assoc. Report No. 3 Review Committee (Member)

J.F. Ely

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

Gas Processors Assoc. Data Book Revision Committee (Member)

AIChE/DIPPR Technical Committee 802 (Member)

NBS/NEL Technical Evaluation Committee (Member)

H.J.M. Hanley

NBS Research Advisory Committee (Member)

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)

AIChE/DIPPR Viscosity Subcommittee (Member)

W.M. Haynes

1985 Cryogenic Engineering Conference Program Committee (Member)

R.D. McCarty

AIChE/DIPPR Vapor Pressure and Density Subcommittee (Member)

J.C. Rainwater

Boulder Editorial Review Board, NBS-Boulder (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, and Standard Reference Materials Subcommittee (Member)

Iota Sigma Pi, Credentials Committee, Women's Honor Society in Chemistry (Member)

American Chemical Society, Fuel Division (Membership Chairperson)

J.G. Hust

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

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

CODATA Task Group on Transport Properties (Member)

International Thermal Conductivity Conference (Member of Governing Board)

R. Radebaugh

Federal Government Interagency Panel on Refrigeration (Member)

Cryogenic Engineering Conference Board (Finance Chairman)

NBS-Cosponsored Conference on Cryocoolers--1984 (Conference Chairman)

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

Organizing Committee for Rocky Mountain Chapter of North American Thermal Analysis Society (Member)

N.A. Olien

ASTM D-3 Gaseous Fuels (Member)

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

IUPAC Committee on Transport Properties (Corresponding Member)

EDITORSHIPS

H.J.M. Hanley

NBS Journal of Research (Boulder Editor)

Physics Today, January 1985 (Guest Editor)

International Journal of Thermophysics (Editorial Board)

W.M. Haynes

Cryogenics (U.S. Editor)

M.J. Hiza

Fluid Phase Equilibria (Editorial Board)

J.G. Hust

Review of Scientific Instruments (Editorial Board)

Journal of Thermal Insulation (Editorial Board)

J.D. Way

Journal of Membrane Science, Proceedings of the Membrane Separation Technology Symposia at the 1983 Denver AIChE Meeting, in press (Guest Editor)

9. PROFESSIONAL INTERACTIONS

FACULTY APPOINTMENTS

J.F. Ely
Adjunct Associate Professor, Department of Chemical and Petroleum Refining Engineering, 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

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

INDUSTRY

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

Consultation with J.P. Frazier, Chairman, Pipeline Research Committee, American Gas Association, Natural Gas Pipeline Company of America, Lombard, IL, on LNG custody transfer.

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

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.

Consultation with L. Lynch, Syntex Chemical Corp., Boulder, CO, on the donation of four reactor tanks, 30 to 1000 gallons, and the use thereof.

G.J. Hanna
Collaborative experimental research with S. Sikdar, General Electric Co., Schenectady, NY, on separation processes and particle size measurement of emulsion liquid membranes.

Consultation with N.N. Li, UOP Inc., Des Plaines, IL, on directions of membrane research.

Consultation with R.M. Laine, SRI Inc., Menlo Park, CA, on facilitated transport in gas and liquid systems.

M.J. Hiza
Consultation with L.D. Wiener, Mobil R&D, Dallas, TX, on equity in transfer of LNG.

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.

Consultation with S.C. Paspek, SOHIO R&D, Cleveland, OH, on stirred tank chemical reactor problems.

Consultation with L. Sobel, Products Chimiques Ugine Kuhlman, Paris, France, CODATA, on 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.A. Waitzman, Tennessee Valley Authority, Muscle Shoals, Alabama, on coal gasification.

K.M. Larson

Collaborative experimental research with S. Sikdar, General Electric Co., Schenectady, NY, on separation processes and particle size measurement of emulsion liquid membranes.

Consultation with P. Mattison, Henicez Corporation, Minneapolis, MN, on complexing agents in separation processes.

Consultation with R. Busche, DuPont Corp., Wilmington, DE, on acetic acid recovery.

D.B. Mann

Collaborative Research with C.R. Sparks, Southwest Research Institute, San Antonio, TX, research at NBS-Boulder Gas Mass Flow Facility for pulsing flow and possible resonance in gage lines.

Consultation with F.W. Sullivan, Chairman, GRI 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, GRI, Chicago, IL, on flow metering research.

S.E. McManus

Collaborative research with C. Griffis, GRI, Chicago, IL, on the decay of turbulent, compressible swirling flow in long pipes.

Consultation with N. Nee, DANTEC Electronics, Franklin Lakes, NJ, on laser doppler anemometry and seeding techniques to measure velocity profiles in turbulent incompressible flow.

R.D. Noble

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

C.F. Sindt

Consultation with W. Siedl, 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 J. Jones, Gulf Research, Houston, TX, on natural gas flow measurement.

J.D. Way

Collaborative research with S. Sikdar, General Electric Co., Schenectady, NY, on separations processes.

Cooperative research with U. Bonne, 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, on properties of petroleum fractions and coal liquids.

Technical Manager of industrial consortium, consultation with member companies involved: Air Products and Chemicals, Inc., Allied Corporation, Amoco Production Company, ARCO Transportation Company, Cooper Energy Services, E.I. DuPont DeNemours and Company, Gas Processors Association, Mobil Research and Development Corporation, Monsanto Company, Phillips Petroleum Company, Shell Development Company, SOHIO, Ingersoll-Rand Company.

Cooperation with staff of the Gas Processors Association and the Gas Research Institute on fluid properties predictions.

H.J.M. Hanley

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

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

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

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

J.C. Rainwater

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

J.E. Callanan

Consultation with S.C. Mraw, Exxon Corporate Research, Annandale, NJ, on thermal measurements on coal.

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

J. Hord

Consultation with W. Wildhaber, Martin-Marietta, Littleton, CO, on solidification of hydrogen in space environment venting.

Consultation with R. Kramarsic, private consultant, Albuquerque, NM, on temperature measurement in high-velocity gas flow.

Consultation with J.J. Fitzpatrick, H.W. Fisher, and V.O. Weed, Rockwell International, Pittsburgh, PA, on gas flow measurement.

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 SRMs.

R. Radebaugh

Consultation with W. Lawless, Ceram Physics, Westerville, OH, on low temperature thermal properties of ceramics.

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.

N.A. Olien

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

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

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

Consultation with H. Brainerd, ARCO Transportation, on custody transfer of CO_2.

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

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 J. Rogers, Los Alamos National Laboratory, Los Alamos, NM, on heat transfer.

Consultation with L. Silvester, Lawrence Berkeley Laboratory, Berkeley, CA, on computer program for transient hydrodynamics.

J.A. Brennan
Consultation with E. Jenkins, California State Dept. of Agriculture, Division of Measurement Standards, on flow measurement standards.

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

Cooperative research with Y. Kuroda, National Aerospace Laboratory, Kakuda Branch, Japan, on cryogenic flow measurement.

D.E. Daney
Cooperative research with L.P. Purtell, Chemical Process Metrology Division, NBS-G in modeling of fluid tangential vortex motion in cylindrical tanks in near zero gravity for mechanically induced transfer between tanks.

P.J. Giarratano
Consultation with M. Young, NBS/Boulder, on transient heat transfer (optical techniques).

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

Collaborative research with A. Cezairliyan and A. Miller, Division 774, NBS, Gaithersburg, MD, on thermophysical measurements in reduced gravity.

Consultation with R.C. Hendricks, NASA-LeRC, Cleveland, OH, on transient heat transfer (boiling in thin liquid films and lubrication).

D.M. Ginley
Collaborative research with S-J. Khang, University of Cincinnati, Cincinnati, OH, on bench-scale mixing tests.

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

G.J. Hanna

Cooperative research with A.L. Bunge, Chemical and Petroleum Refining Engineering, 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.

M.J. Hiza

Consultation with E.D. Sloan, Colorado School of Mines, Golden, CO, on research plans for natural gas hydrate samples.

Consultation with T.H.K. Frederking, University of California, Los Angeles, CA, on AIChE Committee 13H work.

Consultation with W.B. Streett, Cornell University, Ithaca, NY, on thermodynamics of fluid mixtures.

Consultation with R.H. Sherman, Los Alamos National Laboratory, Los Alamos, NM, on phase equilibria of hydrogen and helium isotopes.

Consultation with P.C. Souers, Lawrence Livermore National Laboratory, Livermore, CA, on hydrogen isotope properties for fusion energy.

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

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

Consultation with F. Howard, NASA-KSC, J.F. Kennedy Space Center, FL, on refrigeration/liquefaction costs and solubility data.

K.M. Larson

Cooperative research with A.L. Bunge, Chemical and Petroleum Refining Engineering, Colorado School of Mines, 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.

B. Louie

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

D.B. Mann

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

Consultation with P. Galison, Department of Physics, Stanford University, Stanford, CA, on nuclear physics instrumentation.

S.E. McManus

Collaborative research with P. Purtell, Division 775, NBS, Gaithersburg, MD, on hot wire anemometer and pitot tube techniques for flow measurement.

Collaborative research with W. George, Director of the Turbulence Research Laboratory, State University of New York at Buffalo, Buffalo, NY, on flow measurement at high pressure of swirling flows.

R.D. Noble

Cooperative research with R.G. Bushman, University of Wyoming, Laramie, WY, on mathematical modeling of transient transport phenomena models.

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

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

Consultation with P.C. Wankat, Purdue University, Lafayette, IN, on chemical separations.

Cooperative research with B.E. Dale, Colorado State University, Fort Collins, CO, on immobilized enzyme reactors.

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

J.M. Persichetti

Consultation with E.D. Sloan and A.L. Bunge, Colorado School of Mines, Golden, CO, on hydrodynamic instabilities, primarily dealing with thesis work of Persichetti.

C.F. Sindt

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

J.D. Way

Cooperative research with C.A. Koval, Chemistry Dept., University of Colorado, 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, Chemical Engineering Dept., University of Colorado, Boulder, CO, on facilitated transport using ion exchange membranes.

T.J. Bruno

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

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

D.E. Diller

Cooperative research with L. Van Poolen, Calvin College, Grand Rapids, MI, on measurements of viscosity in liquefied hydrocarbon gases.

J.F. Ely

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

Cooperative research with A. Mansoori, University of IL, Urbana, IL, on local composition models for fluid thermodynamic behavior.

Cooperative research with K.R. Hall, 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, Colorado School of Mines, Golden, CO, on thermal conductivity of coal liquids.

Consultation with F. Zeleznik, NASA-Lewis Research Center, Cleveland, OH, on thermodynamic properties of synthetic jet fuels.

J.R. Fox

Consultation with H.C. Andersen, Stanford University, Stanford, CA, on supercooled atomic liquids and glasses.

H.J.M. Hanley

Cooperative research with E.D. Sloan, A.J. Kidnay, and V. Yesavage, Colorado School of Mines, Golden, CO, on thermal conductivity of coal liquids.

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

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

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

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

Consultation with W. A. Wakeham, Imperial College, London, England, on transport phenomena.

Cooperative research with N. A. Clark, 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.

Cooperative research with staff of the Department of Physics, University of Wroclaw, Poland, on theory of liquids.

W.M. Haynes

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

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

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

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

R.D. McCarty

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

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

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

J.C. Rainwater

Collaborative research with S. Hess, Technical University of Berlin, West Germany, on theory of non-Newtonian liquids.

Cooperative research with M.R. Moldover, NBS, Githersburg, MD, on thermodynamics of near-critical binary mixtures.

Cooperative research with N. Clark, University of Colorado, Boulder, CO, and B.J. Ackerson, Oklahoma State University, Stillwater, OK, on structure of simple liquids under shear.

Collaborative research with T. Paszkiewicz and Z. Petru, University of Wroclaw, Poland, on theory of the Weissenberg effect.

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

H.M. Roder

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

Consultation with M.S. Grabowski and E.D. Sloan, Colorado School of Mines, Golden, CO, on thermal conductivity of fluids.

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

G.C. Straty

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

J.W. Bransford

Consultation with M.C. Branch, Department of Mechanical Engineering, University of Colorado, Boulder, CO, on combustion of metals.

Consultation with D. Pippen, White Sands Test Facility, White Sands, NM, on oxygen safety procedures.

Consultation with C. Byrant, NASA-Kennedy Space Center, FL, on oxygen safety procedures.

J.E. Callanan

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

Consultation with R.W. Carling, Sandia, Livermore, CA, on solid fuels thermal measurements.

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

Consultation with R. Weir, Royal Military College, Kingston, Canada, on solid fuels thermal measurements.

Consultation with J. Crelling, Southern Illinois, University, Carbondale, IL, on solid fuels thermal measurements.

J. Hord

Consultation with A. Powers, DoE, Solar Energy Research Institute, Golden, CO, on microbial photosynthetic production of hydrogen.

J.G. Hust

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

Cooperative research with G.K. White, CSIRO, Australia, on standard reference data research on metals.

Consultation with F. Cabannes, CNRS, France, on low conductivity SRM research.

Consultation with M.L. Minges, WPAFB, Dayton, OH, on standard reference materials and standard reference data research.

Consultation with T. Faison and B. Rennex, NBS, CBT, Washington, DC, on thermal insulation standard reference materials.

R. Radebaugh

Consultation with G. Walker, Calgary University, on low temperature refrigeration.

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

L.L. Sparks

Consultation with R. Barkley, University of Colorado, 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 L.A. Belfiore, Colorado State University, Ft. Collins, CO, and Solar Energy Research Institute (SERI), Golden, CO, on characterization of expanded plastics.

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

S. A. Sullivan

Cooperative research with M.B. Kasen, Fracture and Deformation Division NBS, Boulder, CO, on resin content of polymer composites.

N.A. Olien

Consultation with K.R. Hall, Texas A&M University, on properties of fluids and orifice metering of natural gas.

Consultation with K.E. Starling, Oklahoma University, Norman, OK, on equation of state.

R.O. Voth

Consultation with R.S. Carter, Center for Radiation Research, NBS, Gaithersburg, MD, on helium refrigerator capacity for cold neutron program application.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

Will host a Symposium on Current Status and Future Trends in Thermophysical Property Research at the AIChE Spring National Meeting in Houston, TX, March 24-28, 1985. Organized and Chaired by N.A. Olien and M. Klein (GRI).

Hosted a Rocky Mountain Chapter/AIChE Laboratory tour (60 people) through the Chemical Engineering Science Division on Mar. 20, 1984.

Hosted a tour of the Pharmaceutical Manufacturer's Association (125 people) through the Chemical Separations Laboratory and the Chemical Mixing Laboratory on Mar 8, 1984.

Hosted and co-sponsored the Third Cryocooler Conference at NBS, Boulder on Sept. 17-18, 1984; attended by 150 people from the U.S. and many other countries; co-directed by R. Radebaugh.

Hosted and co-sponsored the Interagency Conference on Cryocoolers (restricted to U.S. citizens) at NBS, Boulder on Sept. 19, 1984; 64 participants; organized and chaired by R. Radebaugh.

WORKSHOPS

Hosted a short course on Data Analysis, Apr. 16-18, 1984, at NBS, Boulder, CO. Attended by Chemical Engineering Science Division staff. Organized by Dr. T. J. Bruno and taught by Charles Hendrix of Union Carbide.

Hosted a workshop on Measurement of Low Concentration Level of Water Vapor in Industrial Gases, Dec. 15, 1983, at NBS, Gaithersburg, MD. Organized and chaired by M. J. Hiza.

Hosted a CPI Measurement Needs Planning Workshop, Apr. 10, 1984, at NBS, Gaithersburg, MD. Attended by selected participants from industry and government. Organized and chaired by J. Hord.

SEMINARS

Professor Z.M. Galasiewicz, University of Wroclaw, Wroclaw, Poland: Kinetics of Phase Transitions and Theory of Viscoelastic Behavior of Fluids and the Construction of a Viscometer, Oct. 3, 1983.

Professor C.N. DeCastro, Instituto Superior Tecnico, Lisbon, Portugal: Thermophysical Properties of Heavy Hydrocarbons, Oct. 5, 1983.

Mr. Paul Dotson, Department of Chemical Engineering, University of Wisconsin, Madison, WI: Brownian Dynamics, Oct. 13, 1983.

Professor J.J. Christensen, Chemical Engineering Department, and Professor R.M. Izatt, Chemistry Department, Brigham Young University, Provo, UT: Separation of Metals by Membranes Containing Macrocyclic Carriers, Oct. 13, 1983.

Dr. J.G. Calvert, Senior Scientist, National Center for Atmospheric Research, Boulder, CO: The Chemistry of Acid Rain Generation, Nov. 4, 1983.

Dr. J. King, CPC International, Argo, IL: Extraction and Fractionation Studies Utilizing Supercritical Fluids, Nov. 9, 1983.

Professor D.L. Katz, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI: The Need for Practicing Engineers to Understand Basic Thermo Physical Behavior, Nov. 14, 1983.

Professor W.A. Wakeham, Imperial College, London, England: Thermal Conductivity Measurements in Liquids, Nov. 17, 1983.

Dr. Y.B. Tewari, Chemical Thermodynamics Division, NBS, Gaithersburg, MD: Thermodynamic Studies of Enzymatic Conversion of Glucose to Fructose, Nov. 21, 1983.

Dr. S. Abramowitz, Chemical Thermodynamics Division, NBS, Gaithersburg, MD: Biotechnology in the NBS, Dec. 7, 1983.

Mr. J. Bayless, Chief Deputy District Attorney, Denver, CO: Computer Crime, Dec. 16, 1983.

Ms. P. Phillips, Wardenburg Student Health Center, University of Colorado, Boulder, CO: Nutrition and Cancer, Jan. 27, 1984.

Dr. D.C. Wingeleth, Chematox Laboratory, Inc., Boulder, CO: Chemistry and the Law: Driving Under the Influence, Feb. 3, 1984.

Professor M.C. Jones, Colorado School of Mines, Golden, CO: Convective Motions in Packed Beds, Feb. 10, 1984.

Dr. K.N. Marsh, TRC, Texas A&M University, College Station, TX: Thermodynamics of Multicomponent n-alkane Mixtures, Mar. 2, 1984.

Professor R. Gammon, University of Maryland, Baltimore, MD: Wetting Layer Thickness in Sulfur Hexafluoride, Mar. 9, 1984.

Professor E.L. Cussler, University of Minnesota, Duluth, MN: Two New Liquid Membranes, Mar. 15, 1984.

Dr. R.B. Lehman, Colorado Bureau of Investigation, Denver, CO: The Application of Chromatography of Forensic Science, Mar. 16, 1984.

Dr. G. Beierl, EPA, Region 8 Laboratory, Denver, CO: Mass Spectrometry in Environmental Testing, Mar. 30, 1984.

Dr. G.R. Olhoeft, U.S. Geological Survey, Denver, CO: Petrophysics - The Physics and Chemistry of Rocks and Minerals, Apr. 6, 1984.

Dr. P. Danesi, Argonne National Laboratory, Argonne, IL: Interfacial Kinetics, May 1, 1984.

Professor J.G. Eberhart, Chemistry Department, University of Colorado, Colorado Springs, CO: The Limit of Superheat of Liquids and Liquid Mixtures, May 23, 1984.

Mr. G. Kimura, General Electric Co., Schenectady, NY: Membrane Technology: An Industry View of Research Needs, June 8, 1984.

Dr. S. Angus, Imperial College, London, England: Equation of State and Transport Property Research at the IUPAC Centre, Aug. 3, 1984.

Dr. T.B. Reed, Solar Energy Research Institute, Golden, CO: Biomass Energy - Can it Compete with Coal and Gas?, Sep. 7, 1984.

Dr. R. Perkins, Rice University, Houston, TX: A New Transient Hot-Wire Thermal Conductivity Instrument for use with Step and Ramp Power Forcing, Sep. 21, 1984.

Dr. H. Knapp, Institut fur Thermodynamik und Anlagentechnik FRG, Berlin, West Germany: Experimental Measurements of Phase Equilibria and Caloric Properties of Fluids, Oct. 1, 1984.

Dr. J. Kulijewicz, Ship Research Institute, Szczecin, Poland: Flow Behavior in Concentric Rotating Cylinders, Oct. 11, 1984.

Dr. J.W. Kaakinen, Bureau of Reclamation, Denver, CO: Characteristics of Reverse Osmosis Fouling at the Yuma Desalting Test Facility, Oct. 12, 1984.

Dr. L. Liao, Agrigenetics Corporation, Boulder, CO: Genetic Engineering: Examples in Boulder, Oct. 19, 1984.

Mr. S.B. McCray, Department of Chemical Engineering, University of California, Los Angeles, CA, The Effects of Acetyl Content on the Transport Parameters of Cellulose Acetate Reverse Osmosis Membranes, Oct. 25, 1984.

Dr. J. Crelling, Department of Fuels Engineering, University of Utah, Salt Lake City, UT, Photoacoustic Microscopy of Coal Macerals, Oct. 26, 1984.

TECHNICAL ACTIVITIES
OF THE
THERMOPHYSICS DIVISION (774)

H.J. Raveche, Chief

(Fiscal Year 1984)

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; membrane transport 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

The Statistical Physics 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.

° Dynamic Measurements-Ared Cezairliyan, Technical Leader

The purpose of this program is to develop dynamic (millisecond and microsecond resolution) techniques; perform measurements of selected thermophysical properties of high melting point substances to temperatures over the range 1500-6000 K; probe nonequilibrium phenomena such as superheating; 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 temperatures for prolonged periods and because of long equilibration times.

° 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) to check the validity of proposed theories for interfacial wetting; and (3) develop the spherical acoustic resonator as a state-of-the-art measurement tool for equilibrium and transport properties of gases and gaseous mixtures.

° 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, non-random errors in thermodynamic measurements.

4. SELECTED PROJECT SUMMARIES

Workshop on Supercritical Solvents, OCT. 17-18, 1984

J.M.H. Levelt Sengers, M.E. Paulaitis

Paulaitis and Levelt Sengers organized a 1 1/2-day workshop with one or two invited speakers in each of four areas: phase diagrams, industrial applications, thermodynamic models, and supercritical chromatography. Members of Divisions 773 and 774 gave short presentations in all areas except industrial applications. Although no official announcement of the workshop was made, the number of requests from industry for attendance was rather overwhelming.

We ended up with representatives from oil, chemical, food, and drug industries, some of which volunteered to speak and contributed significantly to the substance and quality of the meeting. Apparently, this workshop was the first at which physical chemists, chemical engineers, and analytical chemists have met to discuss this topic.

Some conclusions of the workshop were that this is a fast-growing area of chemical engineering with potential for application in a variety of industries, and that there will be a strong need for experimental study and modeling of complicated phase diagrams at pressures considerably above usual critical pressures.

Representatives of Divisions 773 and 774 used this opportunity to have a joint session in which each participant sketched his or her work in this area, and in which the opportunities for collaboration were actively explored.

The First U.S.-Japan Joint Seminar on Thermophysical Properties

A. Cezairliyan, J.V. Sengers (U.S. organizers)

The first U.S.-Japan Joint Seminar on Thermophysical Properties was held in Tokyo, Japan in October 1983, under the sponsorship of the U.S. National Science Foundation and the Japan Society for the Promotion of Science. The seminar brought together experts on thermophysical properties research from the two countries for the purpose of promoting information exchange, comparing problems of interest and approaches used for solutions, and fostering mutual cooperation and understanding. Papers were presented by 28 scientists on a wide range of topics related to thermophysical properties, including general review papers on status and trends of research in the two countries. More specific papers covered high temperature solids, fluids at high pressures, high temperature liquids, and novel measurement techniques. A second joint seminar is being planned and will be held in the U.S. in about three years.

Semi-Automated PVT Facilities

D. Linsky, J.M.H. Levelt Sengers, H.A. Davis

Under sponsorship by the Department of Energy Office for Basic Energy Sciences an effort is underway to modernize and automate partially an existing high-quality Burnett PVT facility for work in the range of 0-200°C. A first step in the automation has been the development of an automated pressure injector that keeps a sensitive transducer, which separates the sample gas from a balancing gas, in the null position as the temperature, and therefore the pressure, is changed. This device was designed, built (Waxman, Davis et al.) and put into productive operation. A Review of Scientific Instruments article recently appeared in print, and a patent application has been submitted.

The transducer position is sensed by means of a capacitance bridge; the dependence of the transducer capacitance on the dielectric constant of the balancing gas is canceled by means of a computer-interfaced Varicap in another arm of the bridge.

The PVT facility will be semi-automated. One reference isotherm will be established in manual mode using the Burnett principle. Pressure-temperature relations will be measured automatically, the density being calculated from the reference isotherm data. In manual mode, the pressure is measured on a dead-weight gage. In automated mode, it is measured on a computer-interfaced quartz spiral Bourdon gage. In both modes, the temperature is measured on a platinum resistance thermometer by means of a computer-interfaced 6 1/2 digit DVM.

We have taken data on the vapor pressure of isopentane in the automated mode, and on the cell constant in the Burnett mode. Compared to previous operation, manpower needed to run the apparatus has been reduced by a factor of two, while the data reduction has been taken over completely by the computer.

We are currently, for the first time, taking data on a binary mixture (isobutane-isopentane) with condensable components, and meeting several challenges in preventing unwanted phase separation. A special oven and interfaces with a gas chromatograph have been constructed.

This work was reported in the Proceedings of the 2nd Symposium on Energy Engineering Sciences, April 1984, at Argonne National Laboratories.

Shear Viscosity

B. Berg, M.R. Moldover

A torsion oscillator is being developed to measure the viscosity of fluids at moderate temperatures (0-100°C) and pressures (0-10 MPa) at very low frequencies (0.5 Hz) and very low shear rates (0.05 sec^{-1}). The oscillator will be used in a NASA sponsored project for testing the theory of dynamic critical phenomena. Low frequency, low shear rate viscosity measurements are also needed to help understand structured fluids (microemulsions, polymer solutions, etc.).

Film Balance

G. Morrison, H.A. Davis

The first of three stages in the film balance construction has been completed, e.g., the construction of the thermostated water trough in which the films will be contained. The circulating bath for rough temperature control and the fine temperature controller have already been purchased and are ready for final assembly of the apparatus.

The second part of the balance, the stepping motor mechanism for varying film surface areas, is being designed. Finalized plans for fabrication will be submitted in the near future.

The third part of the balance, the stress sensor and the automation for both data taking and hardware control, is in a development stage. The computer and the data acquisition system with the appropriate hardware and software are presently in place. The stress-gage bridge is being designed and will be fabricated during the next few months.

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-ranged 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 size of 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. A program of experiments to further test this theory has begun.

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 ultra-pure 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 are being 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.

Thermophysical Measurements in Zero-Gravity 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 zero-gravity environment. This system is an extension of the unique facility developed earlier in this laboratory for the dynamic measurement 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 the first phase of this program, experiments were performed to examine the competing effects of gravity, surface tension, and electromagnetic forces on the geometrical stability of a molten specimen. The experiments were conducted by P. Giarratano of the Center for Chemical Engineering in Boulder in a KC135 aircraft operated by NASA which provides a near-zero-gravity environment for a few seconds. The results indicated that the specimen retained its geometry for a brief period after melting. Changes and refinements in the system are underway to improve operation of the system and extend the excursion to considerably beyond the melting point of the specimen.

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 underway. This technique will enable extension of the present capabilities to measurements on high temperature liquid conductors. As a part of the technique, development of methods for accurate measurements of temperature and power, both with microsecond resolution, are essential. A special two-wavelength optical pyrometer has already been constructed for this purpose. During FY-84, progress was made in the accurate determination of electrical power imparted to the specimen. Determination of power is based on measurements of pulse current and pulse voltage every 1 microsecond. Preliminary results indicate that these quantities can be measured with 1% uncertainty, which represents an advance in the state-of-the-art of pulse high-current, high-voltage measurements. During FY-85, development of electrical measurements will be finalized and work towards measurement of heat of fusion of refractory metals will begin.

Thermophysical Properties of Tungsten-Rhenium Alloy Measured

A. Cezairliyan, A.P. Miiller

Heat capacity and electrical resistivity of tungsten - 3 (wt.%) rhenium alloy have been measured in the temperature range 1500-3600 K with the millisecond-resolution pulse heating technique. This alloy is used as a high temperature thermocouple material. A knowledge of its thermal and electrical properties is needed in the assessment of thermocouple operations.

Compendium of Thermophysical Properties Measurement Methods

K. Maglic, A. Cezairliyan, V.E. Peletsky (editors)

The first volume of this unique compendium was published in FY-84. This volume (800 pages) contains 20 chapters on measurement methods for thermal conductivity, thermal diffusivity, heat capacity, thermal expansion, and thermal radiative properties. This work was done, in part, under the U.S.-Yugoslav Joint Board for Scientific and Technological Cooperation. The second volume of the compendium is in preparation.

Thermal Properties of Coal

R.A. MacDonald, R.D. Mountain

A computer program to model the matter loss and heat capacity of coal has been applied to the measurements made by J.E. Callanan and S.A. Sullivan (Division 773) where moisture content of the coal has had significant effect on the results. In our model, we have allowed for the release of adsorbed water, or water bound to inorganic matter, that did not evolve during the normal drying procedure. The results of this calculation are in quite good agreement with experiment. We also explain the markedly different behavior exhibited upon immediate reheating of the sample as the result of the water not requiring any activation energy to extract it from the coal after the initial temperature rise. These results have been communicated at the Gordon Research Conference on Fuel Science and at the 9th European Conference on Thermophysical Properties, and they will be published in the Journal of High Temperatures -- High Pressures. R.A. MacDonald has visited D. Merrick (National Coal Board Staff College, United Kingdom) upon whose work on coal pyrolysis this model is based, to discuss these results. He is very enthusiastic about this work and we are pursuing some of the suggestions he made for verifying certain aspects of the model.

We are currently investigating an aggregate model as a representation of the porous structure in coal. This model will be used for studies of mass transport through the pores and of the effect of pores on the heat capacity. So far, an aggregate model in 2-dimensions has been set up.

Thermal Properties of Solid Gas Hydrates

R.D. Mountain, R.A. MacDonald

We are developing molecular models and the necessary computational techniques to investigate the thermal properties of gas hydrate crystals as part of a DOE sponsored project. Our work complements experimental work in the Chemical Engineering Sciences Division. We have decided on a molecular model for Type I hydrates which is dynamically stable at low temperatures and which has an acceptably small dipole moment. We are in the process of devising computational techniques which will enable us to make rapid, survey type calculations of thermal properties. A collaboration has been established with M.L. Klein of the National Research Council of Canada who is making related studies of the gas hydrates.

Properties of Refrigerant Mixtures

G. Morrison, D. Didion, P. Domanski, M. McLinden, R. Radermacher,
H. Ross (NBS Division 740)

The work this past year can be divided into three parts: measurements, modeling, and promotion.

One of the major problems in the industrial application and the modeling of mixtures of refrigerant materials is the meager amount of reliable information about them. The long range goal of this project is to make measurements on three representative mixtures. The first of these, R13B1 and R152a, was completed except for measurement of the critical region of R13B1 over a year ago. The second, R22 and R114, was completed during this past year. Measurements were made on two-phase systems for the two pure components and seven mixtures which span the composition range at roughly equal spacing. Measurements were made from 15°C to 55°C. No decision has been made about a third mixture; the decision is being delayed because of intense interest by the refrigerant industry in 3-compound mixtures.

A working model was provided to the group in Building Technology in early 1983. Our work since then has involved refinement of the algorithms, refinement of the model, and determination of molecular parameters for as many refrigerants and mixtures as can be found in the literature. During the past year, there have been two major refinements in the algorithms. The first is an algorithm that finds the "best" molecular parameters of any functionally two-parameter equation of state given the saturation information (densities and pressure). The second is an algorithm that finds dew and bubble conditions. The major refinement in the model begun during the past year is to correct for the packing of hard spheres of different sizes in the reference fluid. Finally, with the development of the molecular parameters and dew-bubble algorithms, fitting of thermophysical data to the mixture model has become a relatively straightforward operation; thus a library of equation of state parameters for pure materials and mixtures is being developed (primarily through the efforts of M. McLinden and R.

Radermacher). The original equation of state package for the mixture R13B1 and R152a has been used extensively and successfully by P. Domanski and H. Ross in heat exchanger and cycle modeling.

There are two features about mixtures that we are trying to promote. The first is that an equation of state that treats condensed phases properly will free a user from independent data libraries to estimate the properties of mixtures from those of the pure components. The second is that traditional guessing schemes collapse when conditions are near the critical conditions of one of the constituent components -- even if the mixture is not near critical. G. Morrison has spoken extensively and informally about these phenomena to representatives from several major refrigeration companies (Borg-Warner, Carrier, Trane, etc.) and formally at the ASHRAE (American Society of Heating, Refrigerating and Air Conditioning Engineers) meeting in Kansas City, Missouri in June 1984. G. Morrison will be speaking at meetings in January 1985 and June 1985 on these and related topics to the refrigeration societies.

Modeling of (Dilute) Near-Critical Mixtures

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

The effect of admixtures on near-critical fluids can be dramatic, as has been shown in several recent experiments. These effects are important in engineering applications, such as the estimation of critically-enhanced impurity effects on the density of chemicals in custody transfer, and on the properties of fluids used in Rankine cycles. The properties of supercritical mixtures are of great interest in the growing fields of supercritical extraction and supercritical chromatography.

Four aspects of near-critical binary mixtures have been studied by us in the last year. (1) Global features of phase transitions induced by admixtures into near-critical fluids have been considered. Remarkable effects were reported in several recent experiments on volumes, enthalpies, and specific heat of mixtures with a near-critical component. We have reached a qualitative understanding of these phenomena, and published on this topic in Fluid Phase Equilibria (1984) and a J. Phys. Chem. Letter (1984). (2) Special effects arise in dilute near-critical mixtures, in that partial molar properties become path-dependent. We have modeled this behavior by means of a classical model and by means of the nonclassical (scaled) Leung-Griffiths model. One striking result is that the critical anomalies in the partial volumes and enthalpies can all be predicted from pure-solvent properties and the initial slope of the critical line. Another is that impurity effects on the density of a near-critical fluid at fixed temperature and pressure are not linear in the concentration of the impurity. This work has been reported in the J. Phys. Chem. Letter mentioned. (3) As a special example of a dilute near-critical mixture we have been studying the behavior of salt solutions near the critical point of steam. A chemical engineering graduate student at Maryland University has been attracted to work on this topic. A recent paper by Pitzer et al. extended the Debye-Huckel treatment of such solutions to high temperatures. We claim that effects other than those given by the Debye-Huckel limiting law dominate near the critical point of steam, and that the very striking experimental anomalies noted have the same origin as in non-electrolyte dilute near-critical mixtures. A paper was given at the 10th ICPS in Moscow, USSR. (4) The solubility of substances in supercritical solvents undergoes a marked enhancement near the mixture critical end point. This is one reason for the current strong interest in supercritical solubility. We are modeling this phenomenon by means of classical equations and the Leung-Griffiths model as we did for dilute mixtures. In addition, we are developing a decorated lattice-gas model, in which the mixture model can be mapped onto a pure-fluid model. The idea is to obtain a nonclassical description of the dilute mixture in terms of the pure solvent and a minimum of additional parameters.

This work was reported in talks at the Department of Chemical Engineering Science at Brigham Young University, at the Physics Department at the University of Colorado at Fort Collins, at the Physics Department of the University of Louvain, Belgium, at the 10th ICPS in Moscow, USSR, and at the Department of Chemical Engineering at Texas A&M University.

Phase Equilibrium in the Critical Region of Mixtures

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

In previous work this inter-divisional 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 Anneke 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.

Molecular Dynamics Studies of Fluid Mixtures

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

A molecular dynamics study of the phenomenon of collision induced far infrared absorption in a mixture of liquid Ar and Ne has been made. The initial motivation for the study was to determine whether or not collision induced absorption measurements could be used to measure mutual diffusion processes in mixtures. While our results for this question are negative, they suggest that collision induced absorption is a sensitive probe of intrinsic three body effects in liquids. A report of this work has been published [J. Chem. Phys. 81, 2347 (1984)] and further studies are in progress for p-H_2-He mixtures.

Equilibrium Properties of Polydisperse Fluids

A. Brown, K. Johnson, D. Jonah, J. Kincaid, G. Morrison, J. Salacuse, 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 increase substantially 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 expresses those conditions in terms of two Fredholm determinants, the calculus of which demonstrates that critical conditions may be viewed as a well-controlled limit of the corresponding finite-component conditions. A statistical mechanical treatment of random systems was completed, providing an alternative to the usual polydisperse limit, and preliminary work on a molecular dynamics calculation of the equation of state of polydisperse soft spheres indicates that our previous perturbation calculations for nearly monodisperse fluids may have a wider range of applicability than previously anticipated. We have derived an 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. A generalization to the study of polydisperse mixtures is underway.

Based on a continuing study of the properties of nearly monodisperse fluids, we have discovered a new, highly-efficient method for calculating the dew and bubble curves for mixtures with an arbitrary number of components. The new algorithm shows that the much simpler nearly monodisperse model can be used even when the distribution function describing a polydisperse fluid is quite broad -- when the width of the distribution is roughly half the average peak of the distribution.

A program to construct an automated, variable-volume visual VLE cell to provide benchmark data on pentane-like multicomponent systems is underway. This data will be used to test polydisperse models. The apparatus is nearing completion; most of the experimental problems have been overcome and a series of measurements on the bubble pressure of n-butane over a range of temperature (320-345 K) has shown that reproducible and internally consistent results can be obtained. Recently, the apparatus has been interfaced to a laboratory microcomputer -- this has involved establishing the nature of automation required and developing much of the software needed to perform the tasks. Before measurements can be made on mixtures the sampling system must be tested and the correct conditions for reproducible analysis established. Once this has been completed, measurements will be made on a binary n-alkane mixture before progressing to mixtures of more components whose thermodynamic properties should be described by polydisperse models.

We organized, in collaboration with M. Klein of the Gas Research Institute, the Symposium On Systems With Very Many Components held at the March meeting of the AIChE in Atlanta. The symposium brought together biochemists, chemical engineers, physicists, mathematicians, and chemists to exchange ideas and techniques related to polydisperse systems.

Properties of Working Fluid Mixtures for Binary Geothermal Power Cycles

J.S. Gallagher, J.M.H. Levelt Sengers, D. Linsky, G. Morrison, M. Emeruwa, J.V. Sengers, B. Kamgar-Parsi, J. Rainwater, D.E. Diller, L. Van Poolen

A binary geothermal plant, which will use a 90 mol% isobutane, 10 mol% isopentane mixture as a working fluid, is under construction at Heber, California. Under contract with the Department of Energy, we are developing the data base for the mixture thermodynamic surface required in the design and performance tests of the cycle; also, we are refining predictive techniques for the transport properties of the mixtures. We use a multi-pronged approach. (1) We are measuring the vapor-liquid equilibrium properties, which include bubble -- and dew -- pressure temperatures, compositions, and densities for mixtures of around 90 mol% and 50 mol% of isobutane in the range of 15-125°C. Data in the range 15-125°C were taken before. A chemical engineering graduate from Howard University has been trained this year and is currently taking data in the range of 55-85°C; she will extend the work to 125°C (Morrison, Emeruwa). (2) We have taken vapor pressure data on pure isopentane and are engaged in taking PVT data for the 90-10% mixture by the Burnett method in the range of 150°C (Linsky, Levelt Sengers). (3) We have measured viscosities of several light hydrocarbons and their mixtures in order to test a predictive corresponding-states model for its reliability (Diller, Van Poolen). These results and some of those on modeling described below have all been documented in a final report to the sponsor. (4) On the basis of the accurate thermodynamic surface that we previously developed for isobutane (Waxman, Gallagher), of the available scarce data for pure isobutane, and of the mixture's VLE and critical line data, we (Gallagher, Levelt Sengers) developed a thermodynamic surface by the method of generalized corresponding states using isobutane as reference fluid. We derived the location of the critical line and the phase boundaries from the model. Tables of thermodynamic properties and a large-size P-H chart have been prepared as an interim report to the sponsor. These results were presented by Gallagher at the August 1984 annual meeting of Geothermal Resources in Reno, Nevada. (5) Finally, we have made a first attempt at constructing an accurate scaled representation of the mixture near the critical line, a region that is of interest in the actual power cycle involved. Although we have encountered some difficulties, these are currently being resolved in a collaborative effort of Divisions 773 and 774 (J.V. Sengers, J.M.H. Levelt Sengers, J. Rainwater, B. Kamgar-Parsi).

Two NBS Internal Reports, elaborated versions of the reports to the sponsors, are currently in NBS review.

The plan is to refine the thermodynamic surfaces when the data-taking is completed, and to merge it properly with the critical-region surface.

Acoustic Cavitation and Ultrasonic Chemistry

J.R. Dorfman, J. Hubbard, F. Martinez, J. Mercer, L. Schmid

The objective of this work is to provide a theoretical and experimental study of the effects of high intensity, low frequency sound on chemical reactions in liquids. Ultrasonic chemistry possesses several distinct advantages over conventional chemical methods. In contrast to initiation by heating, sonolytic chemistry does not require a significant increase in the liquid temperature, and compared to radiolysis or photolysis, the scaling problems are straightforward.

The physical mechanism of sonolysis has become the subject of considerable speculation. It is now generally agreed that, depending on the physical conditions, the ultrasound either produces highly unstable gas vacuoles whose implosion generates transient hot spots with local temperatures and pressures up to several thousand degrees Kelvin and hundreds of atmospheres, or stable, resonating gas bubbles are produced, the radial oscillations of which give rise to considerably milder conditions than in the transient case. We have constructed phenomenological models for describing the thermodynamics and chemical kinetics associated with an isolated collapsing or pulsating bubble. In collaboration with M. Sheer, W. Braun, and M. Kurylo, two experiments have been designed to probe the thermal conditions inside a stable, gas-filled pulsating bubble. The first utilizes the decomposition kinetics of cyclobutanone as a chemical thermometer; the second is laser induced fluorescence spectroscopy of hydroxyl radicals formed in the sonolysis of water.

Also, a study has been made of the feasibility of injecting bubbles of chemically reactive gases and aerosols into a fluid in an ultrasonic resonator in order to induce implosions -- this should produce high-temperature, high pressure chemical reactions of the reagents contained within the bubbles. This study has also examined the feasibility of using purely fluid-dynamical means in the form of pumps and diffusers to induce the desired implosions of the bubbles.

Theory of Solvated Ion Dynamics and Molecular Motions in Polar Liquids

J. Hubbard, S. Lee, J. Rasaiah, P. Stiles, P. Wolynes

The primary objective of this research is to provide quantitative insight into the fundamental mechanisms which determine the transport properties of electrical charges in polar fluids. In addition, the continuum version of these theories is of sufficient generality so as to be applicable to any kind of rigid body motion of an arbitrary charge distribution in a dielectrically dispersive medium. It has recently been proved (by other workers) that this theory of electrohydrodynamics constitutes a rigorous generalization of linearized viscous hydrodynamics and classical electromagnetism, and as such it predicts a novel class of coupled transport phenomena, the experimental consequences of which have only begun to be investigated. A definitive exposition of these theories has just been completed and will appear as a chapter in the book "The Physics of Ionic Solvation," which is part of a series devoted to modern electrochemistry and electrophysics.

A novel mechanism for dielectric relaxation in an inhomogeneously polarized liquid has been proposed. This is a natural generalization of Debye's theory of rotational diffusion to include the translational motions of polar molecules. This analysis has already had a significant impact in interpreting picosecond relaxation spectroscopy data for fluorescence decay and charge transfer reactions in polar liquids. We have also just begun what we hope will be the first successful molecular dynamics computer simulation of ionic mobility in a polar liquid. This will result in a detailed microscopic picture of ionic transport which should help to answer such questions as the dynamic nature of ionic solvation, and the effects of ion size, charge, and solvent dipole moment on ion mobility.

A conference on electrochemistry in science and industry is being organized at NBS. We plan to invite industrial and university experts from such diverse areas as statistical mechanics and solar energy conversion. The workshop is to provide an environment which actively promotes cross-fertilization and inter-disciplinary research in this rapidly growing field.

Energy and Mass Transport in Mixtures

J.R. Dorfman, J. Kincaid, J. Mercer, L. Schmid, D. Tsai

The purpose of this work is to investigate the basic processes of energy exchange among reacting chemical species, as well as transport properties of non-reacting fluids. These processes are fundamental to our understanding of the rate of chemical reactions and the hydrodynamics of mixtures. With the recent advances in lasers and picosecond chemistry, computer simulation of the energy relaxation processes at an atomistic level has become a vital aid to the interpretation of experiments.

In collaboration with S. Trevino and A. Lowrey, we have extended our molecular dynamics investigation to the system $AB \rightleftharpoons A+B$ accompanied by $B+B \rightleftharpoons B_2$ + energy. The energy distribution and the kinetics of the reactions have been studied in detail. We have also examined the initiation of chemical reactions in a dense explosive and have obtained, for the first time, an atomistic description of the structure of a detonation wave in such a system.

We have determined, in collaboration with E.G.D. Cohen and M. Lopez de Haro, thermal diffusion coefficients of the Revised Enskog Theory for binary and ternary mixtures. Our calculations indicate that accurate values of the thermal diffusion factor require using the fourth or fifth Enskog approximation. Also, we calculated the scattered light spectrum of binary mixtures in the presence of temperature and composition gradients using the method of fluctuating hydrodynamics.

Kinetic Simulation of Aggregation of Particulates

R.D. Mountain, 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. This involves solving a set of stochastic differential equations (Langevin equations for Brownian motion) subject to the condition that whenever two particles touch they stick, forming a growing aggregate. Results have been obtained for the free molecular regime and work is in progress on the continuum limit for the background gas. Initial results were reported at the International Conference on Kinetics of Aggregation and Gelation.

Theory of Fluids and Interfaces

R.F. Kayser, J. Kincaid, G. Morrison, H.J. Raveche, L. Schmid, J.M.H. Levelt Sengers, J.V. Sengers

The purpose of this work is to: (1) develop a fundamentally based model for the calculation and correlation of the thermodynamic properties of fluids and fluid mixtures; (2) advance the theory of critical points and lines; and (3) study concentration profiles in interfaces and applications to systems with polydisperse impurities.

A new correction to the scaling relations for the thermodynamic properties of fluids near their critical point was discovered. The analysis of this new correction was based on the actual behavior of the spatial correlation of two (arbitrarily chosen) molecules in a fluid with realistic interactions. At large intermolecular separations the correlation has the form of the intermolecular potential times the square of the isothermal compressibility. The latter is small in dense systems, but anomalously large near phase transformations such as the gas-liquid critical point. Realistic effects on the potential such as retardation entered the analysis. The possibility exists of observing very unusual critical behavior for fluids with certain power-law potentials, such as the ion-induced dipole interaction. Examples of such systems are molten salts. The work illustrates how the current theory of critical phenomena based on renormalization group methods must be advanced to account for the contributions from long-range forces.

We published an extensive review on the application of the renormalization group theory of critical phenomena to the representation of thermodynamic properties of fluids in the critical region (Int. J. Thermophysics). Our scaled fundamental equation incorporates the correct critical singularities and provides an accurate representation of the critical region for industrially important fluids such as steam (J. Chem. Phys. Ref. Data), heavy steam (J. Chem. Phys. Ref. Data), ethylene (NBS Tech. Note), and isobutane (J. Chem. Eng. Data).

In collaboration with J. Percus, an expression for the surface tension of a fluid containing a polydisperse impurity was derived using a simple local thermodynamic model of nonuniform fluids. Preliminary work was also completed toward extending our variational energy principle for compressible flow in pure fluids to the case of a mixture of gaseous phase chemical reactants with spatially varying mole fractions.

High Temperature Material Properties

R. MacDonald

The purpose of this work is to explore the mechanisms that contribute to the anomalous behavior in the heat capacity of the transition metals. The characterization of these high melting point metals is critical to the aerospace and defense industries.

The specific heat measurements of A. Cezairliyan et al. on the bcc transition metals, V, Nb, Ta, Mo, and W, show a pronounced rise at high temperatures ($T > 1500$ K) that has been often attributed to lattice anharmonicity and the presence of vacancies. We have investigated the effect of anharmonicity by calculating the thermodynamic properties of these metals for temperatures between the Debye temperature and the melting point, using the lattice model that was quite successful for the alkali metals. The results of our calculations are in quite good agreement with experiment for all properties under consideration (thermal expansion, bulk modulus, specific heat) up to 1500 K, but they do not show the steep rise at higher temperatures. We conclude that separate treatment of lattice anharmonicity, as described by lattice dynamical perturbation theory, and static vacancies is not sufficient to describe the heat capacity at the high temperatures in metals such as tungsten. A dynamical treatment of vacancies in an anharmonic lattice is required.

Dimensionless Formulations of Thermodynamic and Transport Properties of H_2O and D_2O

J.V. Sengers, J. Kestin, B. Kamgar-Parsi, J.M.H. Levelt Sengers

In the past year, we have prepared and published (J. Phys. Chem. Ref. Data [1984]) comprehensive packages of the thermodynamic and transport properties of light and heavy water in similar dimensionless forms. These packages were prepared from (1) the dimensioned Haar-Gallagher-Kell formulation for H_2O and Hill-McMillan formulation for D_2O, (2) separate critical-region formulations for both fluids recently published by us (J. Phys. Chem. Ref. Data [1984]), and (3) formulations by J.V. Sengers and collaborators for the viscosity and thermal conductivity of light water (J. Phys. Chem. Ref. Data [1980,1984]).

The dimensionless forms of the Haar-Gallagher-Kell and Hill-McMillan formulations are the ones that have been adopted by the International Association for Properties of Steam. J.V. Sengers has been charged with preparing the releases.

Planning has begun for preparing computer tapes for distribution of these comprehensive packages in collaboration with the Office of Standard Reference Data.

International Standard

L. Haar, J.S. Gallagher

The Haar-Gallagher-Kell (HGK) formulation of the properties of water and steam received approval as the new International Formulation for Scientific Use by the International Association for Properties of Steam at the 10th International Conference in Moscow, USSR, September 1984.

Because of its importance, thermodynamic values for water are the basis of engineering efficiency standards by various engineering organizations. One of these is the International Electrotechnical Commission (IEC) which publishes standards for efficiency and performance criteria for hydraulic pumps and pump turbines. These include thermodynamic standards that extend over only a very limited range. We have shown that HGK is in excellent accord with all measurements in that range, and we point out other advantages to the IEC of adopting HGK for their standard.

The book NBS/NRC Steam Tables, presenting tables and charts of the properties of water and steam in the range 0-30 kilobar, 0-2000°C, was completed and sent to press. It was recently published (Hemisphere/McGraw-Hill).

A Thermodynamic Surface for Carbon-Dioxide and Water

L. Haar, J.S. Gallagher

A thermodynamic surface for the aqueous mixture consisting of water/steam and carbon dioxide has been derived. The derivation is based on an expansion about a molecular model in which the effect of the cross interactions, that is, interactions between unlike molecules are given by the molecular representation. In addition to molecular parameters for the pure components, only one additional molecular parameter is required to represent the mixture. The (empirical) expansion terms refer only to the pure components. An important feature of the derivation is that it reduces identically to the very accurate representations for the pure fluids at the concentration limits.

Thermodynamic Modeling for Mixtures Containing Polar Compounds

L. Haar, J.S. Gallagher

The subject of this program is to obtain a representation for binary mixtures containing water/steam and/or ammonia, which will yield accurate thermodynamic property values over wide ranges of the independent variables. To this end we have developed a molecular based model in which the interaction between unlike molecules (the cross interactions) are given by the molecular representation. In addition to the molecular parameters for the pure components, only one additional parameter is required to represent the mixture. An important feature of the model is that it is designed to be accurate for single phase states over wide ranges of the thermodynamic parameters. Also, the model reduces identically to the very accurate (empirical) representations for the pure components at the concentration limits. This molecular approach represents a major departure from other methods based on corresponding states theories for which parameters are determined with the view of optimizing results for coexisting phases.

5. HONORS AND AWARDS

H.J. Raveche - National Bureau of Standards, Equal Employment Opportunity Award for 1984.

6. PUBLICATIONS

Published

Birnbaum, G. and Mountain, R.D., Molecular dynamics study of collision induced absorption in rare gas liquid mixtures, J. Chem. Phys., Vol. 81, No. 5, pp. 2347-2351 (Sept. 1984).

Cezairliyan, A. and Miiller, A.P., Heat capacity and electrical resistivity of nickel in the range 1300-1700 K by a pulse heating technique, Int. J. Thermophys., Vol. 4, No. 4, pp. 389-396 (1983).

Cezairliyan, A. and Miiller, A.P., Melting temperature of nickel by a pulse heating technique, Int. J. Thermophys., Vol. 5, No. 3, pp. 315-320 (1984).

Cezairliyan, A., A dynamic technique for measurements of thermophysical properties at high temperatures, Int. J. Thermophys., Vol. 5, No. 2, pp. 177-193 (1984).

Chang, R.F. and Doiron, T., Leung-Griffiths model for the thermodynamic properties of mixtures of CO_2 and C_2H_6 near the gas-liquid critical line, Int. J. Thermophys., Vol. 4, No. 4, pp. 337-352 (1983).

Chang, R.F., Morrison, G. and Sengers, J.M.H.L., The critical dilemma of dilute mixtures, J. Phys. Chem., Vol. 88, No. 16, pp. 3389-3391 (Aug. 1984).

Davis, H.A., Low cost tubular sapphire optical cells for study of phase separation in fluid mixtures, Rev. Sci. Instrum., Vol. 54, No. 10, pp. 1412-1413 (Oct. 1983).

Kayser, R.F. and Raveche, H.J., Asymptotic density correlations and corrections to scaling for fluids with non-finite-range interactions, Phys. Rev. A., Vol. 29, No. 2, pp. 1013-1015 (1984).

Kayser, R.F. and Hubbard, J.B., Reaction-diffusion in a medium containing a random distribution of non-overlapping traps, J. Chem. Phys., Vol. 80, No. 3, pp. 1127-1130 (1984).

Kestin, J., Sengers, J.V., Kamgar-Parsi, B. and Sengers, J.M.H.L., Thermophysical properties of fluid H_2O, J. Phys. Chem. Ref. Data, Vol. 13, No. 1, pp. 175-183 (1984).

Kincaid, J.M., Lopez de Haro, M. and Cohen, E.G.D., The Enskog theory for multicomponent mixtures. II. Mutual diffusion, J. Chem. Phys., Vol. 79, p. 4509 (1983).

Kopelman, R.B., Gammon, R.W. and Moldover, M.R., Turbidity very near the critical point of methanol-cyclohexane mixtures, Phys. Rev., Vol. A29, No. 2048, pp. 2048-2053 (1984).

Lopez de Haro, M., Kincaid, J.M. and Cohen, E.G.D., Diffusion coefficients of multicomponent hard-sphere fluid mixtures, ASME Thermophysical Properties of Mixtures, No. 83-WA/HT-46 (Nov. 1983).

Masui, R., Haynes, W.M., Chang, R.F., Davis, H.A. and Sengers, J.M.H.L., Densimetry in compressed fluids by combining hydrostatic weighing and magnetic levitation, Rev. Sci. Instrum., Vol. 55, No. 7, pp. 1132-1142 (1984).

Moldover, M.R. and Gammon, R.W., Capillary rise, wetting layers, and critical phenomena in a confined geometry, J. Chem. Phys., Vol. 80, No. 1, pp. 528-535 (1984).

Moldover, M.R. and Schmidt, J.W., Wetting, multilayer adsorption, and interface phase transitions, Physica 12D, Issue No. 351, p. 359 (1984).

Morrison, G., Anomalies in chemical equilibria near critical points, Phys. Rev. A, Vol. 30, No. 1, pp. 644-646 (July 1984).

Morrison, G. and Kincaid, J.M., Critical point measurements on nearly polydisperse fluids, AIChE J., Vol. 30, No. 2, pp. 257-262 (1984).

Mountain, R., Mulholland, G. and Bukowski, R., Stochastic dynamics simulation of particle aggregation, Proc. of Int. Topical Conference on Kinetics of Aggregation and Gelation, Apr. 2-4, 1984, pp. 83-86 (1984).

Raveche, H.J. and Kayser, R.F., Asymptotic behavior of three-particle correlations, Phys. Rev. A, Vol. 29, No. 2, pp. 1003-1005 (1984).

Salacuse, J.J., Random systems of particles: an approach to polydisperse systems, J. Chem. Phys., Vol. 81, No. 5, pp. 2468-2481 (1984).

Sengers, J.M.H.L. and Linsky, D., Semi-automated facilities for measuring density, PVT and VLE of energy-related fluids, Proc. of 2nd Symp. on Energy Eng. Sci., pp. 17-27 (April 10-11, 1984).

Sengers, J.V. and Sengers, J.M.H.L., A universal representation of the thermodynamic properties of fluids in the critical region, Int. J. Thermophys., Vol. 5, No. 2, pp. 195-208 (1984).

Sengers, J.M.H.L., Morrison, G. and Chang, R.F., Critical behavior in fluids and fluid mixtures, Fluid Phase Equilibria, Vol. 14, pp. 19-44 (1983).

Stiles, P.J. and Hubbard, J.B., Polarization, diffusion and dielectric friction in polar liquids, Chem. Phys., Vol. 84, p. 431 (1984).

Stiles, P.J. and Hubbard, J.B., Electrostriction and dielectric friction on a moving ion, Chem. Phys. Lett., Vol. 105, No. 6, p. 655 (1984).

Trevino, S.F. and Tsai, D.H., Molecular dynamical studies of the dissociation of a diatomic molecular crystal. II. Equilibrium chemical kinetics, J. Chem. Phys., Vol. 81, No. 1, p. 248 (1984).

Waxman, M., Davis, H.A., Horowitz, M. and Everhart, B., An automated pressure regulator, Rev. Sci. Instrum., Vol. 55, No. 9, pp. 1467-1470 (Sept. 1984).

Publications in Progress

Cezairliyan, A., Pulse calorimetry, Chap.: Book, Specific Heat of Solids, Plenum Press (In Press).

Cezairliyan, A. and Miiller, A., Thermophysical measurements on tungsten-3 (wt.%) rhenium alloy in the range 1500-3600 K by a pulse heating technique, Int. J. Thermophys. (Submitted).

Cezairliyan, A., Comment to paper "Measurement of thermodynamic parameters of graphite by pulsed-laser melting and ion channeling", Phys. Rev. Lett. (Submitted).

Gallagher, J.S. and Sengers, J.M.H.L., Thermodynamic properties of isobutane-isopentane mixtures, Transactions of the Geothermal Resources Council (In Press).

Haar, L. and Gallagher, J.S., Thermodynamic values in the vicinity of the specific volume anomaly for water, Proc. of Int. Conf. on the Properties of Steam (In Press).

Hubbard, J.B. and Wolymes, P.G., Theories of solvated ion dynamics, Chap. in Book, Physics of Ionic Solvation, Ed. by J. Ulstrup, North Holland Publishers (In Press).

MacDonald, R.A., Shukla, R.C. and Kahaner, D.K., Thermodynamic properties of BCC crystals at high temperatures I. The alkali metals, Phys. Rev., Vol. B15 (Submitted).

Miiller, A.P., Theory of specific heat of solids, Chap. 1 in Book, Specific Heat of Solids, Vol. I-3 (McGraw-Hill/CINDAS) (In Press).

Miiller, A.P. and Cezairliyan, A., High-speed interferometric method for measuring thermal expansion of solids at high temperatures: Book, Thermal Expansion of Solids (Plenum) (Submitted).

Moldover, M.R., Interfacial tension near critical points and two-scale-factor universality, Phys. Rev. A (Submitted).

Morrison, G., Mixtures of hydrocarbons as polydisperse systems, AIChE Meeting, Symp. on Thermophys. Properties of System with Very Many Components, Atlanta, GA (Mar. 1984) (Submitted).

Mountain, R.D. and Birnbaum, G., Scattering of sound waves by inhomogeneities: time domain analysis, Nondestructive Testing Communications (Submitted).

Olien, N.A. and Raveche, H.J., Thermophysical property data generated by the NBS Center for Chemical Engineering, Proc. of AIChE National Meeting, Aug. 28-31, 1983, Chem. Eng. Prog. Symp. Series (In Press).

Schmidt, J.W., Nielson, M. and Daniels, W.B., Coherent inelastic neutron scattering study of solid orthodeuterium at high pressure, Phys. Rev. (In Press).

Sengers, J.M.H.L., Everhart, C.M., Morrison, G. and Chang, R.F., Impure steam near the critical point, Proc. of 10th Int. Conf. on the Properties of Steam (In Press).

Tsai, D.H. and Trevino, S.F., Simulation of the initiation of detonation in an energetic molecular crystal, Phys. Rev. Lett. (Submitted).

7. TALKS

Salacuse, J., Random System of Particles: An Approach to Polydisperse Systems, Thermophysics Division Colloquium, NBS, Gaithersburg, MD, Oct. 5, 1983.

Cezairliyan, A., A Dynamic Technique for Measurements of Thermophysical Properties at High Temperatures, Fourth Japan Symposium on Thermophysical Properties, Yokohama, Japan, Oct. 21, 1983.

Sengers, J.V., A Universal Representation of the Thermodynamic Properties of Fluids in the Critical Region, Fourth Japan Symposium on Thermophysical Properties, Yokohama, Japan, Oct. 22, 1983.

Cezairliyan, A., Trends in Research on Thermophysical Properties of Solids, U.S.-Japan Joint Seminar on Thermophysical Properties, Tokyo, Japan, Oct. 24, 1983.

Cezairliyan, A., Pulse Heating Techniques for Measurements of Thermophysical Properties at High Temperatures, U.S.-Japan Joint Seminar on Thermophysical Properties, Tokyo, Japan, Oct. 24, 1983.

Sengers, J.V., Transport Properties of Fluids Near a Critical Point, U.S.-Japan Joint Seminar on Thermophysical Properties, Tokyo, Japan, Oct. 25, 1983.

Sengers, J.V., Gravity Effects on Critical Phenomena in Gases, Keio University, Yokohama, Japan, Oct. 28, 1983.

Kincaid, J.M., Polydisperse Models of Petroleum Fluids, Los Alamos National Laboratory, Los Alamos, NM, Nov. 3, 1983.

Hubbard, J., Reciprocal Relations in Electrohydrodynamics, University of Maryland, College Park, MD, Nov. 15, 1983.

Kincaid, J.M., Diffusion Coefficients of Multicomponent Hard-Sphere Fluid Mixtures, ASME, Boston, MA, Nov. 15, 1983.

Kincaid, J.M., The Continuous Spin Ising Model and Euclidean Quantum Field Theory, University of Florida, Gainesville, FL, Nov. 28, 1983.

Mountain, R.D., Computer Simulation Studies of Liquids, Physics Department, Howard University, Washington, D.C., Nov. 30, 1983.

Morrison, G., Research in Refrigerant Mixtures, National Engineering Laboratory, United Kingdom, East Kilbride, Scotland, Dec. 8, 1983.

Kayser, R.F., Asymptotic Density Correlations and Corrections to Scaling for Fluids with Long-Range Forces, 50th Statistical Mechanics Meeting, Rutgers University, New Brunswick, NJ, Dec. 14, 1983.

Berg, R., Sound in Superfluid ^3He, Thermophysics Division Colloquium, NBS, Gaithersburg, MD, Dec. 19, 1983.

Mountain, R.D., Nucleation Studies, NBS Staff Research Seminar, NBS, Gaithersburg, MD, Jan. 19, 1984.

Sengers, J.V., Dynamic Critical Phenomena in Fluids, Technological University, Delft, The Netherlands, Jan. 23, 1984.

Tsai, D., Initiation of Detonation in Dense Explosives, Energetic Materials Division Colloquium, Naval Surface Weapons Center, Silver Spring, MD, Feb. 7, 1984.

Mountain, R.D., Condensed Matter Simulations, Panel for NBS Computing, NBS, Gaithersburg, MD, Feb. 13, 1984.

Tsai, D., Molecular Dynamical Studies of the Energetics of Chemical Reactions in Dense Systems, Physics Department, Howard University, Washington, D.C., Feb. 22, 1984.

Moldover, M.R., Wetting, Multilayer Adsorption, and Interface Phase Transitions, Physics Department, University of Virginia, Charlottesville, VA, March 1, 1984.

Sengers, J.V., Critical Fluctuations in Gases in the Presence of Gravity, University of Maryland, College Park, MD, March 6, 1984.

Kincaid, J.M., Surface Composition in Polydisperse Fluids, AIChE National Meeting, Atlanta, GA, March 12, 1984.

Morrison, G., Phase Equilibrium in a Hydrocarbon-like Polydisperse Fluid, AIChE National Meeting, Atlanta, GA, March 13, 1984.

Berg, R., Sound in Superfluid ^{3}He, Institute for Physical Science and Technology, University of Maryland, College Park, MD, March 20, 1984.

Sengers, J.V., Transport Properties of Fluids in the Critical Region, IUPAC Commission I.2, Imperial College, London, England, March 27, 1984.

Schmidt, J.W., Wetting Phenomena in Binary Fluid Mixtures, Fluids Experimental Facility, NASA, Huntsville, AL, March 28, 1984.

MacDonald, R.A., Thermodynamic Properties of the Alkali Metals at High Temperatures, American Physical Society Meeting, Detroit, MI, March 29, 1984.

Sengers, J.M.H.L., Near-Critical Dilute Mixtures -- Classical and Non-Classical, Department of Chemical Engineering Sciences, Brigham Young University, Provo, UT, March 29, 1984.

Moldover, M.R. (with J.W. Schmidt), Wetting, Prewetting, and Interface Phase Transitions, meeting of the American Physical Society, Detroit, MI, March 30, 1984.

Mountain, R.D., Molecular Dynamics Studies of Crystal Nucleation, Conference on Statistical Mechanics, University of California, Davis, CA, March 30, 1984.

Kayser, R.F., Diffusion and Trapping in Random Media, University of California Conference on Statistical Mechanics, Davis, CA, March 31, 1984.

Kayser, R.F., Decay of Particle Correlations in Fluids, University of California Conference on Statistical Mechanics, Davis, CA, March 31, 1984.

Sengers, J.M.H.L., Dilute Near-Critical Mixtures, Physics Department, Colorado State University, Fort Collins, CO, April 2, 1984.

Cezairliyan, A., Advances in Dynamic Techniques for Thermophysical Measurements at High Temperatures, International Conference of High Temperature and Energy Related Materials, Santa Fe, NM, April 3, 1984.

Morrison, G., Reflections on Critical Behavior in Mixtures, Chemical Engineering Science Division NBS, Boulder, CO, April 3, 1984.

Mountain, R.D. (with G. Mulholland), Brownian Dynamics and Aggregation, Kinetics of Aggregation Meeting, Athens, GA, April 3, 1984.

Sengers, J.M.H.L., Dilute Near-Critical Mixtures, Chemical Engineering Science Division, NBS, Boulder, CO, April 3, 1984.

Sengers, J.V., Thermophysical Properties of Fluids in the Supercritical Region, American Chemical Society, St. Louis, MO, April 9, 1984.

Sengers, J.V., Gravity Effects on Critical Fluctuations in Gases, American Chemical Society, St. Louis, MO, April 9, 1984.

Sengers, J.M.H.L., Semi-Automated Facilities for Measuring Density, PVT and VLE of Energy-Related Fluids, Second Symposium on Energy Engineering Sciences, Argonne, IL, April 10, 1984.

Moldover, M.R., Interfacial Tension and Two-Scale-Factor Universality: A Metacorrelation, Thermophysics Division Colloquium, NBS, Gaithersburg, MD, April 12, 1984.

Berg, R., 5 MHz Attenuation and Phase Velocity Measurements in Liquid ^{3}He-A Over a Wide Pressure Range, American Physical Society, Washington, D.C., April 23, 1984.

Tsai, D., Model Studies of the Initiation of Detonation in Dense Energetic Materials, Spring Meeting of the American Physical Society, Washington, D.C., April 26, 1984.

MacDonald, R.A., Thermodynamic Properties of Cubic Metals, Solid State Seminar, University of Maryland, College Park, MD, April 30, 1984.

Tsai, D., Molecular Dynamics Studies of Energy Transport and Energy Sharing in Dense Systems, a series of 8 lectures and 10 workshop sessions, Institute of Mechanics, Chinese Academy of Sciences, Beijing, People's Republic of China, May 22-June 1, 1984.

Tsai, D., Molecular Dynamics Studies of Energy Transport in Dense Systems, Department of Mechanical Engineering, two lectures, Xian Jiao Tong University, Xian, People's Republic of China, June 4-5, 1984.

Mountain, R.D., Molecular Dynamics Techniques, Brock University Physics Department, St. Catherines, Ontario, Canada, June 13, 1984.

Tsai, D., Molecular Dynamics and Studies of Energy Transport in Dense Systems, Physics Department, Suzhou University, Suzhou, People's Republic of China, June 15, 1984.

Morrison, G., Research in Refrigerant Mixtures, American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) National Meeting, Kansas City, MO, June 20, 1984.

Raveche, H.J., Opening Address of the Conference on the Forefronts of Large-Scale Computational Problems, NBS, Gaithersburg, MD, June 25-27, 1984.

Haar, L., The NBS/NRC Steam Tables, International CODATA Conference, Jerusalem, Israel, June 27, 1984.

MacDonald, R.A., Effect of Water Loss on the Heat Capacity of Coal, Gordon Research Conference on Fuel Science, New Hampton School, New Hampton, NH, July 3, 1984.

Moldover, M.R., The Sigma Xi-squared Problem, Workshop on Interfaces and Wetting, Aspen Institute for Physics, Aspen, CO, July 20, 1984.

Johnson, K.A., Excess Functions Near the Liquid-Liquid Critical Point of (Menthanol + Cyclohexane), Thermophysics Division Colloquium, NBS, Gaithersburg, MD, July 24, 1984.

Moldover, M.R., Observations of Wetting Phase Transitions, Workshop on Interfaces and Wetting, Aspen Institute for Physics, Aspen, CO, Aug. 3, 1984.

Johnson, K.A., Excess Functions Near the Liquid-Liquid Critical Point of (Methanol + Cyclohexane), Chemical Engineering Science Division Colloquium, NBS, Boulder, CO, Aug. 6, 1984.

Berg, R., Modern Viscosity Techniques, Norwegian Technical Institute, Trondheim, Norway, Aug. 13, 1984.

Cezairliyan, A., Advances in High-Temperature Pulse Calorimetry, IUPAC Conference on Chemical Thermodynamics, McMaster University, Hamilton, Ontario, Canada, Aug. 14, 1984.

Miiller, A.P., Measurements of the Heat Capacity of Graphite in the Range 500-3000 K by a Pulse Heating Method, IUPAC Conference on Chemical Thermodynamics, McMaster University, Hamilton, Ontario, Canada, Aug. 14, 1984.

Johnson, K.A. (with M.B. Ewing and M.L. McGlashan), The Liquid-Liquid Critical State of (Cyclohexane + Methanol), IUPAC Conference on Chemical Thermodynamics, McMaster University, Hamilton, Ontario, Canada, Aug. 15, 1984.

Berg, R., Velocity and Attenuation of 5 MHz Sound in Superfluid ^{3}He-B, LT-17 Conference, Karlsruhe, Federal Republic of Germany, Aug. 18, 1984.

Berg, R., Pressure Scaling of Zero Sound in ^{3}He-A from 2 to 31 Bar, LT-17 Conference, Karlsruhe, Federal Republic of Germany, Aug. 18, 1984.

Berg, R., NMR in Bulk ^{3}He-A: Pressure Dependence and Thermometry, LT-17 Conference, Karlsruhe, Federal Republic of Germany, Aug. 20, 1984.

Moldover, M.R., Optical Studies of Interfaces, Exxon Research and Engineering Company, Clinton Township, NJ, Aug. 27, 1984.

Gallagher, J.G., Thermodynamic Properties of Isobutane-Isopentane Mixtures, 1984 Annual Meeting of Geothermal Resources Council, Reno, NV, Aug. 28, 1984.

Sengers, J.M.H.L., Dilute Near-Critical Mixtures, Physics Department, University of Louvain, The Netherlands, Aug. 29, 1984.

Sengers, J.V., Transport Properties of Fluids in the Critical Region, 10th International Conference on the Properties of Steam, Moscow, Union of Soviet Socialist Republics, Sep. 3, 1984.

Haar, L., Thermodynamic Values Near the Critical Point of Water, 10th International Conference on the Properties of Steam, Moscow, Union of Soviet Socialist Republics, Sep. 4, 1984.

Sengers, J.V., Viscosity of Mixtures of Liquid H_2O and D_2O, 10th International Conference on the Properties of Steam, Moscow, Union of Soviet Socialist Republics, Sep. 4, 1984.

Sengers, J.M.H.L., Impure Steam Near the Critical Point, 10th International Conference on Properties of Steam, Moscow, Union of Soviet Socialist Republics, Sep. 5, 1984.

Haar, L., Thermodynamic Values in the Vicinity of the Specific Volume Anomaly for Water, 10th International Conference on the Properties of Steam, Moscow, Union of Soviet Socialist Republics, Sep. 6, 1984.

Cezairliyan, A., Thermophysical Properties of Graphite Above 1500 K, 9th European Conference on Thermophysical Properties, University of Manchester Institute of Science and Technology, Manchester, United Kingdom, Sep. 19, 1984.

Edwards, T.J., Pictures at a Transition: The Measurement of the Specific Heat C_v of CO_2 at the Critical Point, Physics Department, University of Delaware, Newark, DE, Sep. 19, 1984.

MacDonald, R.A., Thermodynamic Properties of BCC Metals, 9th European Conference on Thermophysical Properties, Manchester, United Kingdom, Sep. 19, 1984.

MacDonald, R.A., Effect of Water Loss on the Heat Capacity of Coal, 9th European Conference on Thermophysical Properties, Manchester, United Kingdom, Sep. 20, 1984.

Sengers, J.M.H.L., Dilute Near-Critical Mixtures, Department of Chemical Engineering, Texas A&M University, College Station, TX, Sep. 27, 1984.

Sengers. J.V., Transport Properties of Fluids Near a Critical Point, Texas A&M University, College Station, TX, Sep. 28, 1984.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

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)

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)

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)

H.J. Raveche

Board of Trustees for the Conference on Forefronts of Large-Scale Computational Problems and co-organizer of FF84 which was held at NBS, June 25-27, 1984.

J.M.H.L. Sengers

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

Gordon Conference 1985 on the Physics and Chemistry of Liquids (Chairman)

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 Water and 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

Book, Specific Heat of Solids, McGraw-Hill

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 (Co-editor)

J.V. Sengers

Physica A (Member, Editorial Board)

International Journal of Thermophysics (Member, Editorial Board)

9. PROFESSIONAL INTERACTIONS

ACADEME, NATIONAL LABORATORIES AND GOVERNMENT

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.G. Wolynes, University of Illinois, on preparation of a monograph on solvated ion dynamics.

Collaboration with P. Stiles, MacQuarrie University, Australia, on development of a new theory of dielectric relaxation in which both rotation and translation of dipoles is considered.

Collaboration with D. Huckaby, Texas Christian University, on development of a mathematical model for a random walk that is confined to a random channel with absorbing barriers.

Collaboration with B.U. Felderhof, Institute fur Theoretische Phys., Aachen, Germany, on electrohydrodynamics of charged particles in solution.

Collaboration with R. Noble, NBS, Boulder, on diffusion through membranes for chemical separations processes.

Collaboration with B. Miller, Texas Christian University, on positronium annihilation in liquids near their critical point: correspondence on ergodic behavior of systems with long range interactions.

J.M. Kincaid

Collaboration with B. Hafskjold, SINTEF, Norway, on polydisperse impurities in crude oil.

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), and E.G.D. Cohen and M. Lopez de Haro of Rockefeller University, on kinetic theory.

Collaboration with J.K. Percus, Courant Institute, N.Y.U., on theories of interfaces.

R.A. MacDonald

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

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

M.R. Moldover

Collaboration with A. Voronel, University of Tel Aviv, 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.

Collaboration with J. Rainwater, NBS, Boulder, on thermodynamic models near liquid-vapor critical lines.

R.D. Mountain

Collaborative research with T.A. Litovitz and C.J. Montrose of the Catholic University of America, on liquid state problems.

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

L. Schmid

Cooperative research with D. Frazier and B. Facemire of the NASA Space Flight Center, on binary miscibility-gap system.

J.W. Schmidt

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

J.M.H. Levelt Sengers

Cooperative research with R.T. Jacobsen and M. Jahangiri, University of Idaho, on thermodynamic properties of ethylene.

Cooperative research with P. Clancy of Cornell, B. Gammon of Bartlesville DOE, and J. Mehl of the University of Delaware, on virials of ethylene.

Cooperative research with G. Olchowy, B. Kamgar-Parsi and J.V. Sengers, University of Maryland, on critical behavior of ethylene, light and heavy water, isobutane, and mixtures of isobutane and isopentane.

Cooperative research with J. Kestin, Brown University, on dimensionless recommended correlations of thermophysical properties of light and heavy water.

Cooperative research with R. Masui, National Research Laboratory of Metrology, Japan, and W.M. Haynes, NBS, Boulder, on building and testing of magnetic densimeter.

Cooperative research with P. Hill of the University of British Columbia, J. Straub of the Technical University of Munich, and K. Watanabe of Keio University, on critical parameters of light and heavy water.

Cooperative research with J.J. Christensen, Department of Chemical Engineering Science, Brigham Young University, on interpretation of supercritical excess enthalpy data (with G. Morrison).

Cooperative research with J. Rainwater, NBS, Boulder, on the thermodynamics of near-critical mixtures of isobutane and isopentane.

D.H. Tsai

Collaboration with S.F. Trevino of the U.S. Army Armament Research and Development Command, and the Radiation Division of NBS, on molecular dynamical studies of the structure of a detonation wave in an energetic molecular crystal.

Collaboration with A.H. Lowrey, Laboratory for Structure of Matter, U.S. Naval Research Laboratory, on molecular dynamics simulation of the decomposition of energetic materials.

10. CONFERENCES, WORKSHOPS AND SEMINARS

CONFERENCES

First U.S.-Japan Joint Seminar on Thermophysical Properties, held October 1983 in Tokyo, Japan. Co-organized by A. Cezairliyan and J.V. Sengers.

AIChE Winter National Meeting, Symposium on Thermophysical Properties of Systems with Very Many Components, held March 11-14, 1984, in Atlanta, GA. Co-organized by G. Morrison and J.M. Kincaid.

Conference on the Forefronts of Large-Scale Computational Problems, held June 25-27, 1984, at NBS, Gaithersburg, MD. Co-organized by H.J. Raveche.

9th Symposium on Thermophysical Properties, to be held June 1985 in Boulder, CO. A. Cezairliyan and J.V. Sengers, organizing committee members.

Gordon Conference on the Physics and Chemistry of Liquids, to be held Aug. 19-23, 1985 in Holderness, NH. J.M.H. Levelt Sengers, Chairman.

WORKSHOPS

Workshop on Supercritical Solvents, held Oct. 17-18, 1984 at NBS, Gaithersburg, MD. Organized by J.M.H. Levelt Sengers and M.E. Paulaitis.

SEMINARS

M. Jahangiri, Center for Applied Thermodynamic Studies, University of Idaho: A New Equation of State for Ethylene, Oct. 6, 1983.

P. Meakin, DuPont Research, Wilmington, DE: Computer Simulation of Fractal Aggregates, Oct. 25, 1983.

S. Chandrasekhar, Raman Research Institute, Bangalore, India: Recent Work on the Physics of Liquid Crystals -- A Review, Oct. 27, 1983.

M. Horowitz, Department of Electrical Engineering, Stanford University: Noise Sources in Wiring for Sensitive Bridges, Parts I and II, Dec. 19-20, 1983.

M. Horowitz, Department of Electrical Engineering, Stanford University: Capacitance Bridges in Magnetic Densimetry, Dec. 28, 1983.

P. Boudjouk, Department of Chemistry, North Dakota State University at Fargo: Ultrasonic Experiments in Fluids, Jan. 20, 1984.

O. Barnea, Biomedical Engineering Science Institute, Drexel University: Temperature and Pressure Measurement, Control and Automation, Parts I and II, Jan. 26-27, 1984.

Y. Rabin, Department of Chemistry, University of California at Los Angeles: Time-Lags in Nucleation Close to the Critical Point, Feb. 3, 1984.

J. Kestin, Division of Engineering, Brown University: The Problem of Choking in Two-Phase Flow, Feb. 8, 1984.

L. Reichl, Department of Theoretical Physics, University of Texas at Austin: Field-Induced Chaos in Non-Linear Systems, Feb. 9, 1984.

S.A. Rice, University of Chicago: Structure of the Liquid-Vapor Interface of a Metal, Feb. 15, 1984.

F. Kohler, Ruhr-Universitat, Bochum, West Germany: Thermodynamic Properties of Liquids and Liquid Mixtures Based on a Generalized van der Waals Equation of State, Mar. 6, 1984.

R. Koningsveld, DSM Research and Patents, Holland: Small Molecules and Large Molecules, Differences and Similarities in Thermodynamic Behaviour, Parts I, II, and III, Mar. 6-8, 1984.

J. Deutch, Massachusetts Institute of Technology: Diffusion-Limited Aggregation, Mar. 15, 1984.

E. Dickenson, Department of Food Science, Leeds University, United Kingdom: Polydisperse Fluids and Colloidal Suspensions, Mar. 16, 1984.

O. Indekeu, University of Rhode Island: Discussion of Thin Fluid Layers Near Critical End Points, Mar. 20, 1984.

A.G. Schlijper, Shell Research B.V., The Netherlands: A New Pseudo Component Concept for Equation-of-State Calculations, Apr. 13, 1984.

M.H. Ernst, Institute of Theoretical Physics, University of Utrecht, The Netherlands: Transport Properties of a Hopping Model with Strong Disorder, Apr. 25, 1984.

P.T. Cummings, Chemical Engineering Department, University of Virginia: Analytic Solutions of Integral Equations for Molecular Fluids, Apr. 26, 1984.

M.C. Marchetti, University of Maryland: Anomalous Diffusion of Charged Particles in a Strong Magnetic Field, May 2, 1984.

B. Widom, Cornell University: Reflections on the Ising-Model Interface, May 8, 1984.

J. Lipa, Physics Department, Stanford University: What's New at the Wavelength-Point? May 10, 1984.

M.N. da Ponte, College of Engineering, New University of Lisbon, Portugal: Thermodynamic Properties of Relatively Simple Liquid Mixtures, May 15, 1984.

D.S. Cannell, University of California at Santa Barbara: Static and Dynamic Scaling for Linear Flexible Polymers, May 16, 1984.

G.H. Findenegg, Institute of Physical Chemistry, Ruhr University, Bochum, W. Germany: Experimental Study of Semicritical Interfaces, June 21, 1984.

G.A. Chapela-Castanaris, Universidad Autonoma Metropolitana Iztapalapa, Mexico: Molecular Dynamics of Continuous Potentials, July 12, 1984.

T. Kragas, Department of Chemical Engineering, Rice University, Houston: Studies of Phase and Volumetric Behavior of Coal Liquid Constituents and their mixtures, Parts I and II, July 19-20, 1984.

D.M. Stillo, Department of Chemical Engineering, Lehigh University, Bethlehem, PA: Laser Doppler Anemometry in Fluidized Bed Columns, July 23, 1984.

W.A. Wakeham, Imperial College of Science and Technology, London: Measurement of Thermal Conductivity of Liquids at High Pressures, July 30, 1984.

R. Renuncio, University of Oviedo, Spain: Chemical Thermodynamics Research in Universities of Madrid and Oviedo, Aug. 10, 1984.

G.M. Schneider, Department of Chemistry, University of Bochum, Federal Republic of Germany: Physico -- Chemical Principles of Fluid Extraction, Aug. 29, 1984.

F.J. Van Kann, Physics Department, University of Western Australia: The Development of a Cryogenic Gravity Gradiometer, Sep. 4, 1984.

J.D. Weeks, Bell Laboratories, Murray Hill, NJ: Fluctuations at Interfaces, Sept. 24, 1984.

TECHNICAL ACTIVITIES OF THE CHEMICAL PROCESS METROLOGY DIVISION (775)

J.J. Ulbrecht, Chief

(Fiscal Year 1984)

1. INTRODUCTION

The consolidation of the Fluid Engineering Division and the Thermal Processes Division into a single Chemical Process Metrology Division in 1982 created a potential for a research unit endowed with expertise in the metrology of some of the basic process variables typical of the chemical and process industries, such as flow rate, temperature, density, chemical composition, and others.

Under the leadership of Acting Division Chiefs, M.M. Hessel, M.J. Hiza, and H.G. Semerjian, the new Division has steadily expanded its scope of expertise while maintaining some of the traditional research patterns in the areas of turbulence and combustion. The fundamental studies of vortex shedding meters, the development of laser tomography, the work on specialized fiber optic probes are some of the success stories of this period.

At the same time, the new Division provided the industry with accurate measurement and traceability to national standards required for equity in trade and international competitiveness through calibrations in the areas of flow, air speed, density, humidity, and volume.

After the initial period of consolidation of the new Division, it became obvious that the integration within this Division cannot be successfully completed without a redefinition of its long term mission and without an internal restructuring of its Groups. The process started gathering momentum after the appointment of the first Division Chief, J.J. Ulbrecht, in May 1984. The driving forces behind the redefinition were, in particular, the need to:

(i) strengthen the orientation of the Division towards the requirements of the chemical and process industries;
(ii) balance the calibration assignments;
(iii) minimize the overlaps among the constituent units;
(iv) balance resources and the use of unique facilities.

The motivation for a new Division structure is in providing the new Groups with a sense of identity based on clearly defined long term goals, and, at the same time, a sense of belonging in a larger unit which results from the many common interests and potential interfaces. The redefinition of the Chemical Process Metrology Division's basic mission and of its long term research plans derived therefrom were completed in August 1984 and the new organization implemented in October 1984.

With due consideration given to the overall mission of the Center for Chemical Engineering and to missions of the other two Divisions, the Chemical Process Metrology Division sees the following four major thrusts of research as constituting its mission:

(i) fast chemical reactions in homogeneous flows, particularly in mixing jets and vortex sheets;

(ii) multiphase flows with and without chemical reaction at ambient temperatures with particular emphasis on slurry, polymerization, and biochemical reactors;

(iii) reacting flows at high temperatures, such as oxidation, hydrogenation, and cracking;

(iv) sensing of generic variables common to all processes.

Further, the calibration work needs to be firmly based in a sound scientific environment.

Thus, effective from October 1, 1984 the following four Groups were established:

Fluid Flow: The mission of this 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 and liquids with particular emphasis on the mixing flows with fast chemical reactions in jets and vortex sheets.

The Group is also responsible for the provision of accurate and reliable calibration services for flowmeters and anemometers.

Further, the Group is charged with the development of the calibration services for two-phase and multiphase flows.

Multiphase Reacting Flows: The mission of this Group is to study multiphase flow at ambient and near ambient temperatures with and without chemical reactions with the view of developing measurement techniques and fundamental data to improve understanding and control of physical and chemical processes in low temperature chemical reactors, in particular for biochemical, slurry, and polymerization reactors. Because of the rheologically complex behavior of these systems, the investigation of on-line viscometric techniques is an integral part of the overall effort.

High Temperature Reacting Flows: The High Temperature Reacting Flow Group is concerned with the study of catalytic and non-catalytic chemical reactions carried out at elevated temperatures, particularly those involving dispersed particles either formed during the process (combustion in flames) or entrained (fixed and fluidized beds). The purpose of these studies is to develop advanced measurement techniques and to provide fundamental data to improve understanding and control of high temperature reactors.

Process Sensing: The Process Sensing Group performs research directed toward the development of new chemical and biochemical process measurement techniques and methods. Specifically, it is concerned with the measurement of key process parameters utilizing a variety of physical, physicochemical, and biochemical sensing techniques and their combinations.

The interaction between the processes taking place in the vicinity of the sensor, the processes at the sensor's interface, and those controlling the signal transmission are of particular interest.

Substantial effort is devoted to the development of techniques for the assessment of data consistency.

Additionally, the Group is responsible for the development of basic standards for volumetric, density, and humidity measurement and for the use of these to provide accurate and reliable calibrations.

2. GOAL

Within the framework of the Center for Chemical Engineering, the domain of the Chemical Process Metrology Division's main concern is the science of measurement in reactive flows.

The mission of the Chemical Process Metrology Division is to provide the chemical engineering community in industry, government agencies, and academia with expertise in process measurement and modeling. In particular, the work of the Division concentrates on homogeneous and heterogeneous flow systems with and without chemical 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 environment of the sensor with the physical, chemical, and biological transformations taking place in the interface of the sensing element.

It is further recognized that process measurement is a crucial component in 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 on foreign markets.

Parallel with the research work, the Division maintains a state-of-the-art calibration service for flow, volume, density, humidity, and airspeed to improve the international competitive position of the U.S. industry and to assure equity in trade.

3. GROUP FUNCTIONS

° Flow Metrology Group - J.R. Whetstone, Group Leader

The former Flow Metrology Group was responsible for all calibration services offered by the Center for FY 84. These were in the areas of volume, density, humidity, flowrate, and airspeed measurements. The major research areas of the group during the fiscal year were in the areas of (1) measurements in solid-liquid flows, (2) development of databases for flowrate measurement devices, and (3) improvements in the scientific base of calibration related measurements. The reorganization of the Division strongly affected this Group which was the largest in the Division with eighteen full or part-time personnel concentrated in the Fluid Mechanics Building. The effect of the reorganization was to focus its objectives on fluid dynamics and flowrate related measurements. The Group Leader charged with the responsibility for the new Fluid Flow Group is L.P. Purtell. The responsibility for measurements in solid-liquid flows was charged to the Multiphase Reacting Flow Group with the appropriate personnel being assigned to that Group. The remainder of the Group was combined with the Harsh Environment Metrology Group to form the Process Sensing Group and the responsibility for the calibration services for volume, density, and humidity measurements was transferred to this new Group.

An added emphasis on mixing flows with fast chemical reactions and the provision of all flow calibrations is now the responsibility of the new Fluid Flow Group, so that its expanded mission is: to study the fundamentals of fluid flow with the aim of advancing the state-of-the-art in flow metrology and of improving and expanding flow measurement capabilities. Current research includes fundamental mixing and entrainment in jet flows, liquid transfer in a zero-gravity environment, and the stability of vortex shedding meter performance. Plans will soon be developed to expand into the metrology of multiphase flows.

° Fluid and Reactor Dynamics Group - J.M. McMichael, Group Leader
L.P. Purtell, Acting Group Leader

The former Fluid and Reactor Dynamics Group conducted fundamental research on mixing process dynamics, chemically reacting flows, and multiphase flow processes. Theoretical, experimental, and computational studies were directed toward improving instrumentation and measurement techniques, providing fundamental technical data, and developing new physical and mathematical models and new computational methods and codes. Research projects concentrated on the effects of organized motions in shear layers on the characteristics of fluid motion and the resulting mixing dynamics. The restructuring of the Division placed an increased emphasis on multiphase flow systems, ranging from particle-fluid mechanics to rheology, from liquid fluidized beds to stirred tanks and bubble columns.

The Multiphase Reacting Flows Group, headed by Acting Group Leader G. Kulin (after the resignation of J.M. McMichael) is a new Group with a new mission, specifically 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) deposit velocity in solid-liquid pipe flow, (2) drop breakup in mixer-blade flow fields, and (3) bubble generation and behavior near mixer blades. However, concurrently with continued work on existing commitments, we have begun the background activity needed to gradually redirect part of the program toward the new aspects of the mission. Examples are (1) use of the slurry flow apparatus to augment investigations of liquid-solid flow behavior in fluidized beds, and (2) the planning of workshops on on-line rheological measurements and on performance standardization of biochemical reactors.

° Combustion Metrology - H.G. Semerjian, Group Leader

The Combustion Metrology Group conducted research on the development of diagnostics and measurement techniques applicable to high temperature chemically reacting multiphase flow systems. Specific areas of interest included measurement of temperature (gaseous as well as condensed phases), gaseous species concentrations, flow velocity, and particle size and number density. Emphasis had been placed on development of in-situ, real-time, non-intrusive measurement techniques, based on optical/spectroscopic methods. These techniques have been applied to investigation of soot formation in diffusion flames, combustion controls, dynamics of spray combustion systems, pyrolysis and oxidation in two-phase flow reactors, and fluidized bed systems. During the reorganization, the composition of the Group staff has remained relatively unchanged; however, the mission of the Group has been expanded.

The New High Temperature Reacting Flows Group, again headed by H.G. Semerjian, will continue the current effort in combustion and will extend it to the metrology of high temperature (and pressure) reactors, in general. The Group will be concerned with the study of catalytic and non-catalytic chemical reactions carried out at elevated temperatures, particularly those involving dispersed particles either formed during the process (e.g., soot formation during combustion) or entrained into the flow stream (e.g., fixed and fluidized beds, sprays, etc.). The current work on soot formation will be extended to coke formation and deposition on surfaces; the combustion work will include non-oxygen atmospheres and non-carbonaceous fuels, including biomass; and the spectroscopic techniques will be extended to in-situ diagnostics for bioreactors. The objective of these studies will be to develop advanced measurement techniques and to provide fundamental data to improve understanding and control of high temperature reactors.

° Harsh Environment Metrology - K.G. Kreider, Group Leader

The primary emphasis of the former Harsh Environment Metrology Group was to provide measurement science and technology of contact sensors applicable to conditions of extreme temperature and chemical compositions. Work has concentrated mainly on solid state sensors (thin film sensors) with some effort going into optical fiber thermometry.

Considerable overlap developed between the Harsh Environment Metrology Group and the Flow Metrology Group so that it became desirable to form one integrated unit, i.e, the Process Sensing Group. The Group Leader is Dr. J.R. Whetstone with Mr. F.E. Jones as Acting Group Leader until Dr. Whetstone has completed the majority of the work on the API-funded orifice database project. The Process Sensing Group's primary objective is the development of new or improved measurement technologies and procedures for chemical and biochemical processes with particular emphasis on real-time measurements in process environments. A major research effort in the Group is the development of process measurements based on surface and thin film sensing technologies with the surface analytical facility being a major addition to the Division's capabilities. A new direction will be taken during FY 85 into the area of development of on-line measurement techniques for biochemical systems. In addition, the Group is responsible for volume, density, and humidity calibrations.

examining the pressure drop in the horizontal test section as a function of volumetric flowrate (solids plus water). Runs start with flow well above critical and proceed, with incrementally reduced water flow but constant solids flow, through the sliding-bed critical point and into the stationary bed regime. The shape of the curve and location of the pressure-drop minimum are compared with visual observations of the solids flow and bed condition with a view toward contributing to a database for a potential new model. Experiments have been made so far on a 0.55-mm sand; the program will include sand of other diameters and, hopefully, solids of different specific gravity. It is anticipated that this apparatus will provide the data base for subsequent development of slurry flow calibration capabilities.

Solid Phase Distribution Measurement Using X-Ray Tomography*

J.R. Whetstone and D.S. Loebbaka

The simultaneous measurement of the solid and liquid phase concentration and distribution in solid-liquid systems may be accomplished in a non-intrusive 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. However, initial prototype development will utilize non-rotating techniques to obtain sufficient views for phase distribution reconstruction. Initial experiments with the multi-ray detector assembly are expected to be performed during FY 85.

FLUID AND REACTOR DYNAMICS GROUP

Vortex Shedding Flowmeter Research**

G.E. Mattingly and B. Robertson

Vortex shedding flow phenomena -- the basis of operation of the currently very popular flowmeters used in industrial flow process control and in fluid custody transfer applications -- are being investigated to understand generic performance features. This two year project which has been designed collaboratively with vortex shedding flowmeter manufacturers and users is being sponsored by an industry-government consortium formed for these purposes. The objective of the study is to characterize the phenomena known as "jitter and fade" which are observed intermittently in the output signals from these types of flowmeters and which perturb their performance. Our project is designed first to assess and quantify these "jitter and fade" phenomena in the natural flow field about a specially selected vortex shedding strut and then to artificially create this intermittency and to examine its effects using laser Doppler velocimetry (LDV) techniques. This artificial intermittency is created by vibrating the shedding element, a technique directly descended from the vibrating ribbon for the boundary layers developed at NBS in the 1940's. The flow loop, associated instrumentation, and the vibrating element have all been installed and

*Now in Multiphase Reacting Flows Group.

**Now in Fluid Flow Group.

tested for proper performance. The experimental results of our project are being provided to consortium participants through regular meetings and reports and will be published in the technical literature. In addition to flowmeter manufacturers, potential users of vortex meters, such as the NASA Marshall Space Flight Center and the Gas Research Institute, have joined this consortium. Many other firms are currently considering joining.

Jet Mixing Process Dynamics*

L.P. Purtell, T.T. Yeh, R.W. Davis, and E.F. Moore

The entrainment process in the turbulent mixing of a round jet in a coflowing stream is being investigated experimentally and computationally. Acoustic resonances in the air column have been found to influence the formation of vortices within the shear layer but also to provide a convenient mechanism to drive the vortex formation at discrete frequencies. The waves in the early part of the shear layer (which develop into the vortices) have been found to accelerate from one-half the jet speed to an average of the jet and the external stream speeds. This change in scaling characteristics may be accounted for, by using as a characteristic velocity the average of the jet speed and the local minimum speed. These findings are contrary to some published theoretical analyses predicting a simple scaling based only on the average of the jet and external stream speeds. Frequency spectra measured in the shear layer confirm this evolution and scaling. An extensive computational examination of forcing the shear layer (by oscillations in the velocity field) revealed that a particular combination of subharmonic and fundamental frequencies can shed vortices in the shear layer. An examination of shear layer response to turning off the forcing revealed a decay of the oscillations thus implying the absence of any feedback mechanism from the vortices to the early shear layer. All of these mechanisms greatly influence the flowfield and thus its mixing characteristics.

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

K. Yuk and J.J. Ulbrecht

The mechanism of bubble release from the tip of a gas-filled cavity attached to the downstream face of a blade in a rotational shear flow is being investigated. The force on the blade for different rates of aeration, average bubble size, and size distribution are measured. An attempt will be made to correlate the bubble size distribution information obtained from a capillary probe to the flow parameters and fluid properties. The result can be used to predict the interfacial area in agitated reactors, such as fermentors.

*Now in Fluid Flow Group.

**Now in Multiphase Reacting Flows Group.

Current work has focused on rapid measurements in non-symmetric fields at repetition rates up to 10 kHz, using a six angle tomographic approach. The system is operational and is being evaluated by measuring extinction fields 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 seems particularly appropriate for a six angle system, and it will be used in future work.

Flame Temperature Measurements by Laser Excited Fluorescence*

J.J. Horvath and H.G. Semerjian

A new non-intrusive 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 anti-Stokes 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 pre-mixed 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° below the adiabiatic 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 also observed which yielded abnormally high temperatures. To correct for this broad band fluorescence interference, measurements are presently being performed using an optical multichannel detection system which will also allow temperatures to be obtained from a single 10 ns laser pulse. Application of this technique in sooting diffusion flames will complement the data already obtained on the particle and velocity fields.

Particulate and Droplet Diagnostics in Spray Flames*

C. Presser, H.G. Semerjian, and 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 the fuels

*Now in High Temperature Reacting Flows Group.

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 variable-vane swirl burner, which simulates operating conditions found in practical combustion systems. A combination of non-intrusive probing techniques is being utilized to obtain comprehensive data on the spray combustion characteristics, including soot particle and droplet size, number density and volume fraction, gas composition, velocity, and temperature fields. Current efforts are focused on laser scattering measurements for determination of droplet size distribution in the flame, and on high speed cinematography (2,000 - 10,000 fps) for investigation of droplet/gas flow interactions.

Spectroscopic Studies of Levitated Single Particles*

R.E. Preston, T.R. Lettieri**, and H.G. Semerjian

The utility of spontaneous Raman spectroscopy for monitoring chemical composition changes in single aerosol droplets is being investigated. Initial experiments have been carried out using light pressure from an argon ion laser beam to stably levitate 10-35 μm diameter droplets of silicone oil and dioctyl phthalate. All of the Raman peaks of the bulk liquid are found to be present in the spectra of a single droplet of the same liquid. This suggests that an in situ chemical characterization of individual droplets may be possible. The droplet Raman spectra also exhibit sharp, size-dependent features not explained by current models of inelastic light scattering from microspheres. The origin of these features is being further investigated experimentally and theoretically. Possible applications of the Raman technique include compositional studies of multicomponent droplets, time resolved studies of droplet evaporation and surface adsorption, and surface reactions on a droplet in a chemically reacting flow. An electrodynamic balance, which has been assembled in collaboration with Prof. E.J. Davis of the University of Washington, will be used to levitate particles in future studies.

Evaluation of Industrial Furnace Combustion Control Systems*

C. Presser and H.G. Semerjian

Efficient control of furnace combustion processes can be accomplished by continuous monitoring of the concentration of oxygen and/or carbon monoxide in the flue gases, and maintaining a mixture of air and fuel which maximizes the heat release rate and minimizes losses. A study has been completed to evaluate O_2 and CO monitoring systems used for combustion controls and to provide reliable data on their performance, operating range, and accuracy. The study included evaluation of three in situ O_2 and two in situ CO monitoring systems which are applicable to furnace and boiler controls. The project will provide technical information that will allow for cost/benefit analysis of combustion control systems and help expedite

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implementation of combustion control technology by industry. The evaluation of the stack gas monitoring systems has been carried out for ranges of furnace operating parameters such as air-to-fuel mixture ratio, burner firing rate, heat extraction rate, fuel type, combustion air preheat temperature, and cyclic operating conditions, which are based on information gathered on typical operational practices of representative industrial furnaces and boilers. The experiments are performed in the NBS experimental furnace under both natural gas and No. 2 oil firing conditions. An on-line gas sampling/analysis system is used as a reference system for comparative evaluation of the stack gas monitors. The system is used to determine the level of CO, CO_2, O_2, NO/NO_x and total hydrocarbon in the stack gases. Data are also being obtained on the radial distribution of the gases inside the furnace chamber, for different energy extraction rates and different equivalence ratios.

Emission Spectroscopy for Control of Combustion/Gasification Systems*

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

Currently available control techniques for gasifiers, recovery boilers, and other industrial boilers are based on stack gas analysis. In-situ monitoring techniques that are being explored now offer fast response as well as specific advantages in developing control strategies for multiburner systems and for staged combustion systems. The goal of this project is to develop such an in-situ measurement technique that can be applied to a variety of high-temperature reactors.

One application of the current emission spectroscopy work is to the black liquor recovery boiler, where previous optical multichannel analyzer (OMA) data indicated that only line emissions from sodium and potassium are readily observed. The potassium line emissions observed at 405 nm in the recovery boiler tests were confirmed by a series of laboratory tests using a premixed methane/air flame seeded with black liquor or with potassium chloride solution mist. These laboratory investigations also indicated that line emissions due to potassium at the two wavelengths (405.5 nm and 766.5 nm) can be used to estimate the gas temperature by the line intensity ratio technique. Current focus of this project is the development of a portable 4-branched fiber optic probe system. Each branch is provided with an appropriate narrow bandpass interference filter (e.g. 405 nm and 765 nm for K-line emissions and 415 nm and 780 nm for measuring the background continuum emissions for subtraction). Successful application of the 4-color system would demonstrate the potential for developing line-intensity ratio techniques based on emissions from trace elements and compounds that are usually present in a number of practical high temperature multiphase reactor systems, including combustion systems and gasifiers.

Another application of emission spectroscopy has been the OMA of spectra from entrained-flow coal gasifiers. The Mountain Fuel Resources, Inc., coal gasifier pilot plant at Salt Lake City, Utah, has been used to demonstrate, under DOE sponsorship, the feasibility of such diagnostics. Optical access to the interior of the gasifier was gained by means of an optical probe, similar to those developed and used in the NBS fluidized bed. The

*Now in High Temperature Reacting Flows Group.

optical signals, transmitted by the probe from the interior of the gasifier, were split into four beams by means of a 4-branch flexible fiber attached to the probe outside the gasifier. This system allowed simultaneous ratio pyrometry and OMA spectroscopy of gasifier processes. Tests in the gasifier pilot plant demonstrated (a) that the quartz probes provide an excellent means of access into high-temperature industrial reactors, and (b) that the OMA can be used for characterization of emission spectra in gasifiers.

Fundamental Studies of Black Liquor Combustion*

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

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. A high-temperature plug-flow reactor (PFR) is being constructed at NBS which will allow investigations of vaporization, pyrolysis, ignition, and combustion of dilute streams of BL droplets. Gas temperatures and flow velocities in the reactor will simulate those in actual recovery boilers. A prerequisite for studies of BL droplet combustion is the development of techniques for reliable on-demand generation of droplets of specified sizes (diameters of the order of 1 mm). A positive displacement technique has been developed to provide controlled droplet sizes. The technique has been evaluated in a series of experiments with liquids having varying densities and viscosities. In addition, an alternative technique is currently being developed, whereby a piezoceramic crystal is used to squeeze droplets out of an orifice whenever a high-voltage pulse is applied across the crystal.

Prior to operation of the PFR, an auxiliary reactor has been designed and constructed. The function of the auxiliary reactor is to appraise the potential problems associated with: (a) injection of droplets into reactor gas streams; (b) definition of droplet trajectories; (c) design of the droplet/particle collectors in the PFR; and (d) assessment of optical techniques for observation of droplets and particles in high-temperature flow reactors. The auxiliary reactor allows the generation of gas streams up to 4.6 m/s at temperatures exceeding 1250 K.

The flow reactors constructed in this project will also be utilized for investigation of pyrolysis and oxidation characteristics of other fuels, such as coal/water, coal/oil, and emulsified fuels. Techniques to be used for temperature, composition, and particle size measurements in these investigations include high-speed cinematography, fiber optic pyrometry, laser based non-intrusive diagnostics, and gas chromatography.

Optical Measurements in Fluidized Bed Reactors*

A. Macek

A high-temperature fluidized bed reactor is being maintained and instrumented for research toward development of advanced in-situ measurement

*Now in High Temperature Reacting Flows Group.

techniques. The reactor has a square cross-section, 15x15 cm, and has a gas throughput capability of up to 150 cm/sec at temperatures up to 900 °C. The principal advance beyond the state-of-the-art probing of fluidized beds has been the development of an optical probe, allowing observation at one or more arbitrarily chosen locations in the interior of the bed. The apparatus has been used in two tasks, one for temperature measurements and the other for a study of solids movement inside the bed.

The radiometric system, which had previously been used to demonstrate the feasibility of fuel-particle temperature measurements, has been modified, by addition of a bifurcated fiber optic bundle and a set of bandpass filters, resulting in improved versatility and better frequency response. A systematic study has been made of char-particle temperatures with coal samples of different ranks and with an oil coke. The chars of different origins were demonstrated to have different temperatures due to different reactivities. A method was developed allowing the estimation of radiant emissivities of chars. The particle temperature data were used to derive heat transfer coefficients in the fluidized bed.

A second task has been initiated, under DOE sponsorship, with the objective of developing techniques for a study of solids movement in fluidized-bed reactors. The impetus for this study is the importance of the problem of mixing in fluidized beds. The study is based on the fact that a burning particle generates a distinct signal as it arrives at an optical probe location. The fluidized bed has been modified for placement of two optical probes at two locations in the bed. Arrival times of fuel particles, fed onto the top of the bed, have been recorded in a series of experiments in which the two probes were located at different points in the bed. It has been demonstrated that migration of particles from the top into the interior of the bed is affected by the fluidization velocity. Statistical analysis of arrival times at various points in the bed with systematic variation of fluidization parameters, will be used for definition of mixing patterns in the bed.

HARSH ENVIRONMENT METROLOGY GROUP

Chemical Sensor Research*

S. Semancik

Experimental studies will be carried out in the Center's new surface analytical laboratory to provide detailed information on the mechanisms by which chemical species can be detected and quantified using contact process sensors. These sensing devices operate on a variety of physical principles, but in all cases the interaction between the chemical being monitored and an active substrate generates some measurable property change. Surface-sensitive techniques included in our facility will allow the effects of such interactions to be directly characterized, thereby producing basic insights required to improve the selectivity, response, and stability of sensing materials; results from such investigations should also stimulate ideas for entirely new sensing methods.

*Now in Process Sensing Group.

Equipment for the facility has been procured, and present delivery dates indicate that operation should begin during the first or second quarter of FY 85. The system will consist of dual ultrahigh vacuum chambers fitted with instrumentation for x-ray photoemission, secondary ion mass spectroscopy, temperature programmed desorption, and electron diffraction. In-situ electrical measurement hardware has been under development and will also be housed within the vacuum enclosure. This special combination of techniques will permit critical correlations to be made between the chemical and electronic responses of sensor surfaces during adsorption. In addition, gas handling equipment being fabricated at NBS will be used in conjunction with the preparation section of the facility to simulate realistic operating environments.

Initial research efforts have been focused on sensing processes involving simple gases and oxide substrates. Particular emphasis has been given to moisture-surface interactions and a paper dealing with the effects of alkali additives on water adsorption has been submitted for publication.

Optical Fiber Thermometry*

K.G. Kreider

A new sapphire fiber optic thermometer has been constructed this year with simultaneous two color optical detection capabilities. This device has been designed to investigate engineering applications including hot reacting flows and liquid metal temperature measurements. Two-channel (600 and 700 nm) data were investigated to determine effects of tip geometry and coating geometry and the results of this work are being published in the Proceedings of the NBS-ASTM Symposium on Radiation Thermometry. The two-color fiber optic probe was also investigated as a thermometer for high speed melt measurements in an RF induction furnace in a cooperative project with the Center for Materials Science.

Results of our work and a project in the Center for Basic Standards on use of the optical fiber thermometer for precise temperature measurement in black-body melting furnaces indicated the need for controlling the surface scattering properties of the sapphire. We are presently investigating the use of various sputtered coatings as potential high temperature optical coatings for the sapphire light guide to control surface scattering. In addition, we are investigating the adherence and durability of coatings for the blackbody tip.

Thin Film Sensors*

K.G. Kreider and S. Semancik

Thin film sensors are being investigated which will permit improved temperature and composition measurements in chemical process streams. Sputtered thin film thermocouples have been fabricated and evaluated on nickel, cobalt, and iron base alloys which are to have applications in gas

*Now in Process Sensing Group.

turbine and internal combustion engines. Emphasis has been placed on the thin film oxides such as Al_2O_3 used as the electrical insulating layers and diffusion barriers for these sensors. Problems of integrity, adhesion, electrical resistance, and dielectric strength have been related to sputtering conditions and thermal treatments. Electron and optical microscopy together with surface analysis techniques have been used to characterize these films as well as the mechanical and electrical testing. New directions in this work include studying the fabrication of the thin film thermocouples on structural ceramics. An NBSIR, "Advanced Thin Film Thermocouples," has been published and documents the investigation of these sensors for gas turbine applications.

An investigation of IrO_2 thin film pH sensors has also been initiated which would expand the capabilities of in-situ pH sensing to higher temperatures, wider pH ranges, and finer spatial resolution. These sputtered thin film sensors also have the potential for superior sterilization techniques and integration with solid state electronics compared with the glass electrode technology. Other sputtered thin films being investigated include Ta_2O_5, which has superior dielectric properties.

5. HONORS AND AWARDS

H.G. Semerjian - Department of Commerce, Silver Medal, in recognition for his major contributions to fundamental science and applied technology by his development of laser tomographic and optical diagnostic techniques for chemically reacting and combustion processes.

6. PUBLICATIONS

Published

Davis, R.W., Moore, E.F. and Purtell, L.P., A numerical-experimental study of confined flow around rectangular cylinders, Phys. Fluids, Vol. 27, No. 1, pp. 46-59 (Jan. 1984).

Dobbins, R.A., Santoro, R.J. and Semerjian, H.G., Interpretation of optical measurements of soot in flames, "Combustion Diagnostics by Nonintrusive Methods," Ed. by T.D. McCay, Prog. Astronau. Aeronau., AIAA, Vol. 92, p. 208 (1984).

Doering, D.L. and Semancik, S., Summary abstract: orientational ordering of an incommensurate sodium layer on Ru (001), J. Vac. Sci. Technol., Vol. A2, No. 2, p. 893 (1984).

Doering, D.L. and Semancik, S., Orientational ordering in a strongly chemisorbed system: Na/Ru (001), Phys. Rev. Lett., Vol. 53, pp. 66-69 (1984).

Huang, P.H., Adsorptive and desorptive characteristics of water vapor on reinforced perfluorinated film as humidity sensors, Bull. Amer. Phys. Soc., Vol. 29, No. 1, p. 45 (1984).

Jones, F.E., Interpolation formulas for viscosity of air, nitrogen, carbon dioxide, helium, argon, and oxygen, Nat. Bur. Stand. (U.S.) Tech. Note 1186 (Feb. 1984).

Jones, F.E., A tank volume calibration algorithm, Nuclear Materials Management, Vol. 13, No. 1, pp. 16-27 (1984).

Kawase, Y. and Ulbrecht, J.J., Approximate solution to the natural convection heat transfer from a vertical plate, Int. Commun. Heat and Mass Transfer, Vol. 11, No. 143 (1984).

Kawase, Y. and Ulbrecht, J.J., Turbulent mass transfer in the entry region, Int. Commun. Heat and Mass Transfer, Vol. 11, No. 457 (1984).

Kreider, K.G., Semancik, S. and Olson, C., Advanced thin film thermocouples, Nat. Bur. Stand. (U.S.) Interim Report 84-2949 (1984).

Madey, T., Benndorf, C., Doering, D.L., and Semancik, S., Influence of surface additives, sodium and oxygen, on the structure and bonding of H_2O and NH_3 on Ru (001), Proc. of 8th Int. Congr. on Catalysis, Vol. 4, pp. 51-62 (1984).

Mattingly, G.E., Spencer, E.A. and Klein, M., Workshop report on fundamental research issues in orifice metering, Gas Research Institute (GRI) Report No. 84/0190 (Oct. 1984).

McMichael, J.M. and Deutsch, S., Magnetohydrodynamics of laminar flow in slowly varying tubes in an axial magnetic field, Phys. Fluids, Vol. 27, No.1, pp. 110-118, (Jan. 1984).

McMichael, J.M., Purtell, L.P., Davis, R.W. and Moore, E.F., Effect of shear layer instabilities and acoustic modes on vortex formation in a coflowing jet, AIAA Paper No. 84-0420, 22nd Aerospace Sci. Meeting, Reno, NV (Jan. 1984).

Moore, E.F. and Davis, R.W., Numerical solutions for steady natural convection in a square cavity, Nat. Bur. Stand. (U.S.) Interim Report 84-2830 (1984).

Potzick, J.E. and Robertson, B., Long wavelength acoustic flowmeter, U.S. Patent No. 4,445,389 (1984).

Potzick, J., Performance evaluation of the NBS longwave acoustic flowmeter, Rev. Sci. Instrum., Vol. 55, No. 7, p. 1173 (1984).

Presser, C., Semerjian, H.G. and Juberts, M., Evaluation of O_2 and CO monitoring systems for combustion controls, U.S. Department of Energy Report PR/06010-T14 (1983).

Ray, S.R. and Semerjian, H.G., Laser tomography for simultaneous concentration and temperature measurement in reacting flows, "Combustion Diagnostics by Nonintrusive Methods", Ed. by T.W. McCay, Progress in Astronau. Aeronau., AIAA, Vol. 92, p. 300 (1984).

Robertson, B., Flow and temperature profile independence of flow measurements using long acoustic waves, ASME J. Fluids. Engr., Vol. 106, pp. 18-20 (Mar. 1984).

Semancik, S., Summary abstract: the reaction of oxygen and aluminum on Rh(111), J. Vac. Sci. Tech., Vol. A2, No. 2, pp. 886-887 (1984).

Whetstone, J.R., Semerjian, H.G., Gaigalas, A., Potzick, J. and Charagundla, S.R., Advanced sensor development program for the pulp and paper industry, Annual Report, U.S. Department of Energy, PR/06010-T33 (1984).

Publications in Progress

Charagundla, S.R., Macek, A. and Semerjian, H.G., Study of combustion spectra from an entrained-bed gasifier for development of advanced optical diagnostics, Proc. of 1st AR&TD and Surface Coal Gasification and Instrumentation Projects-Contractors Meeting, Morgantown, WV, June 13, 1984 (In Press).

Davis, R.W. and Moore, E.F., Numerical modeling of vortex merging in axisymmetric mixing layers, Proc. of 9th Int. Conf. on Numerical Methods in Fluid Dynamics, Springer-Verlag Lecture Notes in Physics (In Press).

Davis, R.W. and Moore, E.F., A numerical study of vortex merging in mixing layers, Phys. Fluids (Submitted).

Davis, R.W., Finite difference methods for fluid flow, Proc. of Computational Techniques and Applications Conference, Sydney, Australia, Aug. 1983 (In Press).

Dils R.R. and Tichenor, D.A., A fiberoptic probe for measuring rapid temperature fluctuations in combustor exhaust gases, Combust. Sci. Technol. (Submitted).

Hasegawa, S., National basis for accuracy in humidity measurements, Int. Symp. on Moisture and Humidity (Submitted).

Horvath, J.J., Pamidimukkala, K.M., Person, W.B. and Green, A.E.S., Spectroscopic observations of methane-pulverized coal flames, J. Quant. Spectrosc. Radiat. Transfer (In Press).

Huang, P.H. and Whetstone, J.R., Evaluation of relative humidity values for saturated aqueuos salt solutions using osmotic coefficients between 50 and 100 degree C, Proc. of 1985 Int. Symp. on Moisture and Humidity (Submitted).

Jones, F.E., A new laminar flow meter calibration equation, Rev. Sci. Instrum. (Submitted).

Jones, F.E., A new method for estimating diverter value corrections, Int. J. Heat Fluid Flow (In Press).

Kreider, K.G., Optical fiber thermometry, ASTM Spec. Tech. Pub. (Submitted).

Lofquist, K.E.B. and Purtell, L.P., Drag on a sphere moving horizontally through a stratified liquid, J. Fluid Mech. (In Press).

Macek, A. and Bulik, C., Optical measurement of char-particle temperatures in the interior of a fluidized bed combustor, Proc. 20th Int. Symp. on Combustion, The Combustion Institute (In Press).

Macek, A. and Charagundla, S.R., Burning rates of lignite particles at low furnace temperatures, Combust. Sci. Technol. (Submitted).

Macek, A., Optical measurements of char-particle temperatures and radiant emissivities in fluidized-bed combustors, Proc. of 3rd Int. Fluidised Bed Conference, Inst. Energy, London, Sept. 1984 (Submitted).

Mattingly, G.E., Fluid metering research at NBS: new research tools and new opportunities, Proc. of Instrum. Soc. America, Paper No. C.1.84-R767, Houston, TX, Oct. 1984 (In Press).

Pellett, G.L., Charagundla, S.R. and Marshall, R.L., Transient processes in combustion of single submillimeter metal droplets, Proc. of ASME Winter Annual Meeting on Droplet Spray Combustion, ASME, New Orleans, LA, Dec. 9-14, 1984 (In Press).

Potzick, J., On the accuracy of low flowrate calibrations at NBS, J. Instrum. Soc. Am. (Submitted).

Ray, S.R. and Semerjian, H.G., Real-time measurement of temperature and concentration distribution in flames, Proc. of 20th Int. Symp. on Combust., The Combust. Inst. (Submitted).

Santoro, R.J. and Semerjian, H.G., Soot formation in diffusion flames: flow rate, fuel species and temperature effects, Proc. of 20th Int. Symp. on Combust., The Combust. Inst. (In Press).

Semancik, S., Doering, D.L. and Madey, T.E., The interaction of water with Li-predosed Ru (001), J. Vac. Sci. Technol. (Submitted).

Ulbrecht, J.J. and Kawase, Y., Mass and momentum transfer with non-Newtonian fluids in fluidized beds, Chem. Eng. Commun., Vol. 32, Jan. 1985 (In Press).

Ulbrecht, J.J. and Kawase, Y., A new approach for heat and mass transfer in granular beds based on the capillary model, Ind. Eng. Chem. Fundamentals (In Press).

Ulbrecht, J.J. and Patterson, G., Mixing by mechanical agitation, Gordon and Breach, NY, 1985 (In Press).

Whetstone, J.R. and Gaigalas A.K., Measurement of the phase fraction of paper pulp in pipes, AIChE J. (Submitted).

7. TALKS

Davis, R.W., Numerical Modeling of Unsteady Free Shear Flows, Westinghouse Bettis Atomic Power Laboratory, Pittsburgh, PA, Oct. 1983.

Purtell, L.P., Instability and Vortex Development in a Coflowing Jet, American Physical Society, Division of Fluid Dynamics, Houston, TX, Nov. 1983.

Semancik, S., The Reaction of Oxygen and Aluminum on Rh(111), 30th National Symposium of the American Vacuum Society, Boston, MA, Nov. 3, 1983.

Macek, A., Temperature Measurements Inside Fluidized Bed Reactors, Chemical Process Metrology Division Seminar, NBS, Gaithersburg, MD, Nov. 17, 1983.

Semancik, S., The Role of Surface Science Studies in the Measurement of Moisture, Center for Chemical Engineering - NBS Workshop on Moisture Detection, NBS, Gaithersburg, MD, Dec. 15, 1983.

Ray, S.R., The Application of Laser Tomography to Measurements in Chemically Reacting Flow Fields, Center for Applied Mathematics Colloquium, NBS, Gaithersburg, MD, Jan. 4, 1984.

Semancik, S., Techniques for Probing Surfaces, Chemical Process Metrology Division Seminar, NBS, Gaithersburg, MD, Jan. 11, 1984.

Huang, P.H., Adsorptive and Desorptive Characteristics of Water Vapor on Reinforced Perfluorinated Film as Humidity Sensors, Annual Meeting of American Physical Society, Committee on Applications of Physics, San Antonio, TX, Jan. 31, 1984.

Semerjian, H.G., Non-Intrusive Measurements in Chemically Reacting Flows, Chemical Engineering Department, Howard University, Washington, DC, Feb. 17, 1984.

Semerjian, H.G., Low-Level Humidity Measurements, SEMI Analytical Procedures Meeting, Phoenix, AZ, Feb. 28, 1984.

Semerjian, H.G., Non-Intrusive Diagnostics in High Temperature Reacting Flows, Texaco, Inc., Montebello Research Laboratories, Montebello, CA, Mar. 14, 1984.

Macek, A. (coauthor: C. Bulik), Direct Measurement of Char-Particle Temperatures in Fluidized-Bed Combustors, Central States Section Meeting, The Combustion Institute, Minneapolis, MN, Mar. 19, 1984.

Preston, R.E., Reactions on Chemically Modified Tungsten Surfaces, Surface Science Division Seminar, NBS, Gaithersburg, MD, Mar. 22, 1984.

Santoro, R.J. (coauthors: H.G. Semerjian and R.A. Dobbins), Optical Measurements of Soot Formation Processes in Flames, Meeting of the American Physical Society, Detroit, MI, Mar. 26, 1984.

Davis, R.W., Numerical Modeling of Unsteady Free Shear Flows, Department of Mechanical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, Apr. 1984.

Santoro, R.J. (coauthor: H.G. Semerjian), The Effects of Temperature and Fuel Species on Soot Particle Growth in Diffusion Flames, Western States Section Meeting, The Combustion Institute, Boulder, CO, Apr. 2, 1984.

Santoro, R.J., Optical Measurements of Soot Formation Processes in Diffusion Flames, Department of Mechanical Engineering, University of California at Berkeley, Berkeley, CA, Apr. 4, 1984.

Santoro, R.J., Optical Measurements of Soot Formation Processes in Diffusion Flames, Sandia National Laboratories, Livermore, CA, Apr. 5, 1984.

Davis, R.W., Numerical Modeling of Unsteady Free Shear Flows, Naval Research Laboratory, Washington, DC, May 1984.

Kreider, K.G., Fiber Optic Thermometry, Symposium on Applications of Radiation Thermometry, NBS, Gaithersburg, MD, May 8, 1984.

Semerjian, H.G., Gas Temperature Measurements in Combustion Systems, Symposium on Applications of Radiation Thermometry, NBS, Gaithersburg, MD, May 8, 1984.

Santoro, R.J., Soot Formation in Diffusion Flames, NBS Workshop on Flame Radiation and Smoke, Gaithersburg, MD, May 10, 1984.

Mattingly, G.E., Prospects for Research-Based Improvements in Thermal Metering, NBS-DOE-IDHA Workshop on Thermal Metering, Gaithersburg, MD, May 21, 1984.

Davis, R.W., Numerical Modeling of Vortex Merging in Axisymmetric Mixing Layers, Ninth International Conference on Numerical Methods in Fluid Dynamics, Paris, France, June 1984.

Horvath, J.J., Flame Temperature Measurements in Premixed Flames by Collision Redistribution of Laser Excited Levels, McDonnell-Douglas Research Laboratories, St. Louis, MO, June 7, 1984.

Mattingly, G.E., Generic Vortex Shedding Flowmeter Research at NBS, Rosemount Co., Minneapolis, MN, June 13, 1984.

Macek, A. (coauthors: S.R. Charagundla and H.G. Semerjian), Study of Combustion Spectra from an Entrained-Bed Gasifier for Development of Advanced Optical Diagnostics, Morgantown Energy Technology Center, Morgantown, WV, June 13, 1984.

Santoro, R.J. (coauthor: H.G. Semerjian), Soot Formation: Effects of Fuel Structure, Temperature and Pressure, Invited Talk at 1984 AFOSR/ONR Contractors Meeting on Air Breathing Combustion Research, Pittsburgh, PA, June 20, 1984.

Ulbrecht, J.J., Measurement of Extension Viscosity, Ecole Polytechnique, Montreal, Canada, June 25, 1984.

Preston, R.E. (coauthors: T.R. Lettieri, M.J. Bell), Raman Spectroscopy of Single Optically Levitated Droplets, 1984 CRDC Scientific Conference on Obscuration and Aerosol Research, Aberdeen, MD, June 27, 1984.

Semancik, S., The Influence of Alkali Additives on H_2O-Metal Interactions, Gordon Research Conference on Solid State Chemistry, Plymouth, New Hampshire, Aug. 8, 1984.

Horvath, J.J. (coauthor: H.G. Semerjian), Flame Temperature Measurements in Premixed and Diffusion Flames by Collisional Redistribution of Laser Excited Levels, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 14, 1984.

Presser, C. (coauthor: H.G. Semerjian), Evaluation of Industrial Furnace Combustion Control Systems, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 14, 1984.

Ray, S.R. (coauthor: H.G. Semerjian), Real-Time Measurement of Temperature and Concentration Distributions in Flames, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 14, 1984.

Macek, A. (coauthor: C. Bulik), Direct Measurement of Char-Particle Temperatures in Fluidized-Bed Combustors, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 16, 1984.

Hayasaka, H. (coauthors: T.T. Yeh, R.J. Santoro, and H.G. Semerjian), A Systematic Study of Temperature Effects on Soot Formation in Laminar Diffusion Flames, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 16, 1984.

Santoro, R.J. (coauthor: H.G. Semerjian), Soot Formation in Diffusion Flames: Flow Rate, Fuel Species and Temperature Effects, 20th Symposium (International) on Combustion, Ann Arbor, MI, Aug. 16, 1984.

Preston, R.E. (coauthor: J.B. Benziger), Heteroatom Chemistry on Tungsten Surfaces, Annual Meeting of ACS, Philadelphia, PA, Aug. 27, 1984.

Preston, R.E. (coauthor: T.R. Lettieri and H.G. Semerjian), Raman Spectra of Optically Levitated Droplets, Annual Meeting of ACS, Philadelphia, PA, Aug. 28, 1984.

Ray, S.R., Laser Absorption Tomography for High Speed Simultaneous Measurement of Temperature and Concentration Distributions in Flames, Department of Mechanical Engineering, University of California at Berkeley, Berkeley, CA, Sept. 4, 1984.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

S. Hasegawa

ASME PTC 19.18, Committee on Humidity Determination (Member)
ASTM D22, Sampling and Analysis of Atmospheres (Member)
ASTM G3, Durability of Nonmetallic Materials (Member)

J.J. Horvath

Optical Society of America - Teller's Committee (Member)

K.G. Kreider

Advisory Panel, Center for Chemical Electronics, University of Pennsylvania (Member)
ASTM E20, Temperature (Member)
ASTM C30, Composite Materials (Member)
Program Committee, International Conference on Solid State Transducers (Member)
Steering Committee on 1985 International Symposium on Moisture and Humidity (Member)

G. Kulin

ASTM D.19, Main Committee on Water (Member)
Task Group D19.03.03.02 on Velocity Measurement (Chairman)
Task Group D19.03.03.03 on Velocity-Area Methods (Chairman)

A. Macek

Combustion Institute - 20th Symposium (International) on Combustion - Program Subcommittee (Member)

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-14, Measurement of Fluid Flow Using Gravimetric and Volumetric Techniques (Chairman)
ASME Ad Hoc Committee on Vortex Shedding Type Flowmeters (Chairman)
ASME Select 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)
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 (Technical Advisor)

R.J. Santoro

Combustion Institute - 20th Symposium (International) on Combustion - Program Subcommittee (Member)

S. Semancik

NSF Evaluation Panel on Catalysis (Member)

H.G. Semerjian

Combustion Institute - 20th Symposium (International) on Combustion - Program Subcommittee (Member)
ASME Heat Transfer Division, K-11 Committee on Heat Transfer in Fires and Combustion Systems (Member)
NBS Research Advisory Committee (Member)

J.J. Ulbrecht

AIChE International Committee (Member)
AIChE National Programs Committee (Member)
Group 3A-Mixing (Chairman-Elect)
Organizing Committee of the Third Conference on Engineering Rheology, London (Member)

EDITORSHIPS

K.G. Kreider

Academic Press (Editorial Board)

A. Macek

Combustion Science and Technology (Editorial Advisory Board)

G.E. Mattingly

International Journal of Heat and Fluid Flow (Editorial Advisory Board)

J.J. Ulbrecht

Chemical Engineering Communications (Editor)

Collaborative research with G. Rosasco of NBS Center for Basic Standards, on Raman spectroscopy.

Cooperative research with S. Arnold of Polytechnic Institute of New York, on diagnostics of levitated single particles.

R.E. Preston and H.G. Semerjian

Collaborative research with E.J. Davis of University of Washington, on single particle levitation in an electrodynamic balance.

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.

B. Robertson

Collaboration with R.C. Calabrese of the University of Maryland on proposal to Office of Naval Research, on turbulence measurements in dilute polymer flows.

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.

S. Semancik

Collaborative work with T.E. Madey, Surface Sciences Division (NBS-Gaithersburg) on the effects of surface additives in chemisorption systems.

Cooperative work with A. Seabaugh, Semiconductors Materials and Processes Division (NBS-Gaithersburg) on surface electrical measurements.

Collaboration with C.D. Olson, Center for Materials Science (NBS-Gaithersburg) on electron microscopic analyses.

Collaborative work with D.L. Doering, Dept. of Physics, University of Florida, concerning overlayer epitaxy of alkali metals.

H.G. Semerjian

Cooperative research with D. Clay of the Institute of Paper Chemistry, on black liquor combustion and pyrolysis.

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 I. Stockel of University of Maine (Orono), on droplet formation and black liquor combustion.

Invited consultant to NASA Lewis Research Center, on Combustion Fundamentals Research Program.

Cooperative research being developed with J. Katz of Johns Hopkins University, on temperature and particle measurements in high temperature reacting flows.

Consultations with T. Milne and R. Evans of Solar Energy Research Institute, on pyrolysis of lignins in flames.

Consultations witih R. Chawla of Howard University, on kinetics of soot formation in flames.

J.J. Ulbrecht

Collaboration with SUNY, Buffalo, NY, supervision of Theses of A.K. Ghosh and K. Yuk, on bubble mechanics.

Cooperative work with A. Stuempfle, Chemical Weapons Research Establishment (Aberdeen Proving Ground, MD) on sensing.

Cooperative projects with L. Friedman, American Red Cross Research Laboratory, on biosensors.

Cooperative work with B. Dale, Colorado State University (Fort Collins, CO) on biosensors.

J.R. Whetstone

Collaboration with D.S. Loebbaka of the University of Tennessee (Martin) on X-ray tomography for slurry flow solid fraction measurements.

10. CONFERENCES, WORKSHOPS AND SEMINARS

CONFERENCES

Session on Heat Transfer in Fixed and Fluidized Bed Systems at the 22nd AIChE/ASME National Heat Transfer Conference, Niagara Falls, NY, Aug. 1984; organized and chaired by H.G. Semerjian.

Session on Combustion-Generated Particulates at the 20th International Symposium on Combustion, University of Michigan, Ann Arbor, MI, Aug. 1984; co-chaired by H.G. Semerjian.

WORKSHOPS

Hosted workshop on Measurement of Low Concentration Levels of Water Vapor in Industrial Gases at NBS, Gaithersburg, MD, Dec. 15, 1983.

Hosted workshop on Measurement Needs in the Chemical and Related Process Industries at NBS, Gaithersburg, MD, Apr. 10, 1984.

Hosted NBS/ASTM Symposium on Radiation Thermometry, May 8, 1984; organized and chaired by K.G. Kreider.

Hosted Thermal Metering Workshop (with DOE and IDHA), May 21, 1984; organized by G.E. Mattingly.

SEMINARS

J.B. Greenberg, The Technion, Israel Institute of Technology, Department of Aeronautical Engineering, Haifa, Israel: Self-Adaptive Gridding and Stable Operator Splitting Methods for Computing Reacting Flow Systems, Nov. 21, 1983.

F.J. Pierce, Department of Mechanical Engineering, Virginia Polytechnic University, Blacksburg, VA: The Horseshoe Vortex Revisited, Jan. 1984.

D. Cox, Department of Chemical Engineering, University of Florida: Surface Characterization of a Pt-SnO_2 Model Catalyst, Mar. 22, 1984.

Y.M. Timnat, The Technion, Israel Institute of Technology, Department of Aeronautical Engineering, Haifa, Israel: Laser Based Size and Velocity Measurements in Two-Phase Flows, June 29, 1984.

T.J. Mueller, Department of Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, IN: Flow Visualization by Direct Injection, July 10, 1984.

M.R. Rao, Indian Institute of Technology, Department of Chemical Engineering, Bombay, India: Studies of Heat Transfer in Fluidized Bed Reactors, July 17, 1984.

R.T. Yang, Department of Chemical Engineering, State University of New York: Coke Deposition on Particles and Their Regeneration, July 23, 1984.

L. Yap, Princeton University, Department of Mechanical and Aerospace Engineering, Princeton, N.J.: Multicomponent Droplet Combustion, July 24, 1984.

B. Tribollet, Physique des Liquides et Electochimie, Universite Pierre et Marie Curie, Paris: Space and Time Correlations for Mass Transfer Fluctuations in Polymers Solution and Turbulent Flow, Aug. 20, 1984.

A. D'Alessio, Universita di Napoli, Instituto di Chimica Industriale, Naples, Italy: Ensemble Light Scattering Methods for the Characterization of Burning Sprays, Aug. 24, 1984.

A. Lodge, Rheology Research Center, University of Wisconsin: The Stressmeter, Aug. 29, 1984.

J. Spann, University of Arkansas, Physics Department, Fayetteville, AR: Laboratory Study of Single Sulfate Aerosol in an Electrodynamic Balance, Aug. 31, 1984.

E.J. Davis, University of Washington, Department of Chemical Engineering, Seattle, WA: Applications of Single Particle Levitation, Sept. 12, 1984.

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11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1984 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, volume, 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 solid-fluid slurry 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)

chemical engineering; fluid mechanics; fluid properties; process measurements; research; sensors; solid properties; thermophysics; unit operations.

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