NBSIR
86-3059

Center for Chemical Engineering

Technical Activities: Fiscal Year 1986

February 1987

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

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J. Hord, Editor

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Prepared for:

National Research Council (NRC)
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Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1986 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science. They embody: development and improvement of measurement principles, measurement standards, and calibration services such as volumetric and mass flow rates, liquid volume, liquid density, and humidity; generation (via accurate measurements and advanced predictive models) of reliable reference data for thermophysical properties of pure fluids, fluid mixtures, and solids of vital interest to industry; and development of improved correlations, models, and measurement techniques for complex flows, heat and mass transport, mixing, and chemically reacting flows of interest in modern unit operations.

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INTRODUCTION

This document summarizes technical research activities of the Center for Chemical Engineering during Fiscal Year 1986 (October 1, 1985 through September 30, 1986). This Center is one of six such units that compose the National Engineering Laboratory of the National Bureau of Standards. A brief summary of the structure and technical activities of the National Bureau of Standards is given in the introductory portion of this report, along with organizational information on the Center for Chemical Engineering.

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

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

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

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- Building Technology
- Fire Research
- Chemical Engineering

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- Fracture & Deformation
- Polymers
- Metallurgy
- Reactor Radiation

INSTITUTE FOR COMPUTER SCIENCES & TECHNOLOGY

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ORGANIZATION OF THE CENTER FOR CHEMICAL ENGINEERING

- **CENTER FOR CHEMICAL ENGINEERING**
  *J. Hord, Director
  M. Hessel, Deputy Director
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    V. Schrodt, Chief
    - Transport Processes (S. Sikdar)
    - System Dynamics (M. Hiza)
    - Properties of Solids (L. Sparks)
  - **THERMOPHYSICS DIVISION**
    * N. Olien, Chief
    - Equation of State & Statistical Physics (J. Levelt Sengers)
    - *Properties of Fluids (W. Haynes)
  - **CHEMICAL PROCESS METROLOGY DIVISION**
    J. Ulbrecht, Chief
    - Fluid Flow (G. Mattingly)
    - Multiphase Reacting Flow (A. Gaigalas)
    - High Temperature Reacting Flow (H. Semerjian)
    - Process Sensing (J. Whetstone)

*Located in Boulder

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≠≠ University Faculty Appointment
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*** Student "Q" Appt.
# National Research Council Postdoctoral Fellow
° Guest Worker
°° IPA - Intergovernmental Personnel Act
°°° IRA - Industrial Research Associate
† FTT - Full Time Temporary
†† PT - Part Time
††† WAE - Intermittent (When Actually Employed)

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GL-Group Leader

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

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

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

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

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

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

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

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

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

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

TECHNICAL ACTIVITIES
OF THE
CHEMICAL ENGINEERING SCIENCE DIVISION

V.N. Schrodt, Chief

1. INTRODUCTION

Efficient design and operation of plants and facilities in the chemical, biochemical, petrochemical, petroleum, gas and other processing industries are strongly dependent on reliable engineering data and well-documented characterization of process mechanisms. Efficient design and operation enable U.S. industry to compete more effectively in the world marketplace, where intense international competition has focused efforts to improve manufacturing equipment and processes. Furthermore, an increased emphasis on environmental protection has created a need for alternative processes operating with closer tolerances, emphasizing higher yields and internal recycling with separation, so that fewer pollutants are produced. The development of accurate process models, for the design of the newer and more unconventional plants and to improve conventional ones, requires reliable and well documented process characteristics as well as accurate models for the transport operations and dynamics represented within these industrial processes. The work of the Chemical Engineering Science Division is focused on providing the knowledge and understanding needed for the elemental processes, and on advancing the state of the art for transport phenomena models and theory. The key ingredients are: laboratory determination of elemental process mechanisms and characteristics, theoretically based predictive models for subprocesses involving and using complex fluids and solids, and analysis of the dynamics of engineering systems. In addition to contributions related to process design and operation, the work of the Division is 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 strong collaboration with the Thermophysics Division to integrate fluid and solids properties with process mechanisms and models, and with the Chemical Process Metrology Division in flow research. These collaborations include several joint projects sponsored by other agencies, and new ones are being explored.

One of the primary focuses of research in the Division is on industries related to the new biotechnology. For the most part, a thorough and quantitative understanding of the behavior of separation factors and transport mechanisms of these new biochemical systems does not presently exist, especially as these relate to products created by genetic engineering. The complexity of the phenomena involved, and the vast array of products and processes encountered, precludes the possibility of a purely experimental or correlative approach. The approach must be one which includes experiment, theory, and evaluation so as to yield accurate process and related transport phenomena, and facilitates the development of generic predictive models that are applicable to a broad range of biosubstances. The theoretical effort will break new ground in understanding separations at the molecular level, phase equilibria involving multiple phases, biological system behavior, heat and mass transfer, and other unit operations. Experimental efforts include membrane separations of amino acids and two-phase aqueous extractions. Other extensions of the state of the art in separation technology are anticipated in the Division's long range plans.

The research of the Division addresses scientific issues of national interest in which NBS expertise and its impartial position are critical to an acceptable resolution, as with the highly accurate measurement and modeling of the flow of fluids such as natural gas, selected fluid mixtures, and cryogens. Standard Reference Materials are developed for selected thermal properties of certain solid materials of interest to the chemical and related industries. The majority of the effort is directed toward problems of the future. These include, but are not restricted to: 1) transport processes related to the efficient use of gases and liquids such as natural and synthesis gas, methanol, etc., for use as chemical feedstocks and fuels; 2) utilization of more selective separation processes; 3) bioproduct separation/purification technology needed for large scale manufacture of biochemicals; and 4) new techniques for management and disposal of potentially harmful chemical wastes. The strategy is to perform basic research, generic to the science underlying the chemical, biochemical and petrochemical processing industries, which requires the special role of NBS as an impartial national laboratory excelling in measurements and their interpretation. During the past year, the effort in membrane separations research has been expanded to include a project on bioseparations. New work was initiated on heat transfer in supercritical extraction processes and on the use of reaction systems at supercritical conditions to treat hazardous wastes. Plans have been developed to initiate new research projects on thermal transport properties of ceramics and composites, and the field of chemical vapor deposition is of future interest to the Division.

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

2. GOAL

The goal of the Division is to provide evaluated generic engineering design data and elemental process engineering models; standard measurement procedures and test methods; predictive techniques, correlations, computer codes, and underlying theories needed by the chemical and related industries to design, control, and develop new manufacturing 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 modeling and predictive techniques, state-of-the-art measurement techniques, and advanced understanding of elemental process mechanisms. The approach is to conduct research on fundamental concepts, new ideas and phenomena, and predictive models in synergism with experimental programs. The endeavors nurture development of new processing techniques, provide accurate models of transport phenomena, and lead to understanding of advanced engineering concepts. An essential corollary of these efforts is the critical evaluation and correlation of experimental measurement techniques, leading to the development of voluntary standard measurement practices and test methods.

3. GROUP FUNCTIONS

The research of the Division is organized into three technical groups: Transport Processes, System Dynamics, and Properties of Solids.

° Transport Processes - S.K. Sikdar, Group Leader

The Transport Processes Group performs experimental, theoretical, and mathematical modeling research in: membrane processes; separation of gases, solutions and biochemicals; heat transfer; destruction of toxic wastes; and transport processes in microgravity.

° System Dynamics - M.J. Hiza, Group Leader

The System Dynamics Group performs research to provide data, measurement methodology standards, and thermodynamic criteria for the optimum application of fundamental principles in physical process operations--including flow metrology at normal and extreme conditions, fluid management in normal and low gravity, and mass and energy changes in multicomponent, multiphase systems--to support programs of other agencies and industrial trade organizations and to promote efficiency and measurement accuracy in the chemical and allied industries.

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

The experimental and analytical research of the Properties of Solids Group is focused on the thermal properties (thermal conductivity, thermal expansion, and heat capacity) of industrially important solids such as: solid fuels (e.g. coal, oil shale, and gas hydrates), foams, fibers, fiberboards, aggregates, metals, ceramics, composites, and polymers. Work is performed on the ignition and combustion characteristics and rapid oxidation of metal alloys, in an oxygen environment, at pressures up to 20 MPa. Efficiencies and new concepts of refrigeration are studied.

4. SELECTED PROJECT SUMMARIES

TRANSPORT PROCESSES GROUP

Separation by Reversible Chemical Complexation: Data, Mechanisms and Modeling

R.D. Noble, J.D. Way, L.A. Powers, S. Bischke, M.-F. Jin, S.K. Sikdar

Reversible chemical complexation offers important advantages over conventional methods for separating species from gases and liquids. The objectives of this research are 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 this facilitated transport technique in separation processes. The fundamental characteristics of this separation technique are being studied by experimental work on two applications: (1) selective separation of gases by an immobilized liquid membrane consisting of an ion exchange membrane neutralized by an organic base carrier, and (2) selective separation of carboxylic and amino acids by acid and salt-forms of ion exchange membranes.

The experimental part of the program includes measurement of mass transfer fluxes and determination of the mechanisms of transport. The mathematical modeling is employed to develop equations to predict species fluxes and separation factors of one species over another. Gases which have been successfully separated using ethylene diamine-mediated perfluorinated ion exchange membranes are CO_2 and H_2S. Current efforts are being directed toward hydrogen and ethylene. In liquids, transport data are being collected on some carboxylic and amino acids, and the mechanism of transport is being established. The gas separation work is funded by DoE.

Biochemical Separation

R.A. Perkins, G.F. Slaff, B.R. Bateman, D. Steward, S.K. Sikdar

The biochemical separation program is a new initiative in separation research. The major objective of this program is to provide data and understanding necessary for the design of industrial bioseparation processes. Current research activities are focused on the technique of two-phase aqueous extraction as a means of separating proteins from aqueous solutions.

The aqueous two-phase extraction technique is an important alternative to chromatographic methods which are expensive. The experimental work undertaken to provide fundamental data, understanding, and models includes: (1) measurement of protein partition coefficient data for two-phase systems consisting of aqueous solutions of polyethylene glycol, dextran, and salts; (2) measurement of mass transfer coefficients for proteins transferring across the interface; and (3) development of the technique of double exposure holography for the measurement of protein diffusivities. On the theoretical side, a statistical thermodynamic approach is being investigated as a predictive tool for protein partition coefficients. The bioseparation program is collaborative with the University of Arizona and the University of Bombay.

Heat Transfer in Supercritical Fluids

M.C. Jones, P.J. Giarratano, L.A. Powers, J.F. Welch

The precipitation or condensation of solutes from supercritical solvents by heating, a phenomenon known as retrograde condensation, is a promising industrial process. However, data and understanding of retrograde condensation in supercritical mixtures, necessary for design of heat exchange equipment, is seriously lacking. The objective of this program is to study the phenomenon experimentally, and provide mathematical models and/or correlations for the prediction of heat transfer coefficients.

An apparatus has been built for measuring heat transfer data for a number of solutes in supercritical carbon dioxide. Plans exist for the observation of the nucleation mechanisms using optical techniques to aid the interpretations of the heat transfer results. Experiments have begun.

Superfluid Helium Transport in Zero Gravity

V.D. Arp, D.E. Daney, P.R. Ludtke, W.G. Steward

Transferring cryogens in space is an integral part of NASA's space program. For cooling and maintenance of expensive equipment in space, superfluid helium needs to be transferred in a microgravity environment. The NBS approach is to use a centrifugal pump, free of cavitation problems. The objective of this program is to support the NASA mission by providing superfluid helium pumping characteristics, and aid in the fabrication of a prototype for tests on board a space shuttle.

SYSTEM DYNAMICS GROUP

Metering of Natural Gas and Cryogenic Liquids

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

At the core of this work is a flow facility capable of providing accurate and precise mass-based data for flowing cryogenic liquids and ambient temperature gas. There are three projects currently under study. The first is aimed at providing substantial improvement in the metering of natural gas by means of orifice and turbine type flowmeters. This multi-year program, funded by the Gas Research Institute, includes an extensive series of measurements on a 4-inch diameter orifice meter used for interlaboratory comparisons in Europe. Also under investigation are swirl phenomena, flow conditioning concepts, and pipe roughness effects. The work in Boulder on gas flow is closely coordinated with similar work on water flow in the Chemical Process Metrology Division. The second area of flow research utilizes the flow facility to evaluate new measurement techniques and to perform special tests on meters to provide measurement traceability to NBS. These tests are performed with liquid nitrogen. The third area of flow research is concerned with high velocity flows (over 50 m/s) and utilizes water from a local hydroelectric plant since such velocities are well beyond the range available in a laboratory. The purpose of this work is to assist NASA in developing reliable flowmeters for the Space Shuttle Propulsion System.

Process Thermodynamics

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

This work is designed to provide engineering, principally cryogenic engineering, expertise to other government agencies to solve or provide the basis for solution of a variety of problems. Current research is concerned with 1) performing experiments on condensed cryogens and evaluating the thermodynamics of, and heat and mass transfer effects in, systems used in inertial confinement fusion; 2) reviewing and evaluating thermodynamic modeling of cryogenic systems in support of high energy physics experiments at the National Accelerator Laboratory; 3) analyzing the fluid mechanics, thermodynamics, and phase equilibria, and assessing the applicability of measurement methodology in the production, transfer, and storage of liquid-solid mixtures of hydrogen; and 4) performing experiments and analyzing the fluid mechanics and thermodynamics on the transfer and storage of large quantities of fluids such as liquid hydrogen, oxygen, and superfluid helium with application to fluid management in low gravity environments. The work in areas 1) and 2) is supported by the Department of Energy, in area 3) by the Defense Advanced Research Projects Administration, and in area 4) by the National Aeronautics and Space Administration.

PROPERTIES OF SOLIDS GROUP

Solid Fuels Research

J.E. Callanan, B.J. Filla, J.G. Hust, K.M. McDermott, L.L. Sparks, S.A. Sullivan

The techniques developed for measurement of the heat capacity of raw coals have been extended to coals of different ranks, premium coals, chars, and ash. The total enthalpy of an exothermal reaction, observed on the initial heating of a raw coal, has been evaluated. The magnitude of the enthalpy change is related to the degree of oxidation of the coal. Through collaboration with other coal scientists, we will continue our attempts to understand this reaction. Other experimental results which will aid in this evaluation include those for premium coals, for heat capacities studied in various atmospheres, for heats of desorption of water from coal, and the analyses of the effluent gases. Measurements on macerals will permit evaluation of the mineral contribution to the overall reaction. Maceral specimens have been prepared.

The high pressure cells that will be used to extend the measurements of heat capacities above 600 K have been activated and their accuracy and precision evaluated. We will proceed with the higher temperature measurements during the coming year.

A new series of coal-epoxy specimens, with different proportions of the two components, will be prepared on site for use in thermal conductivity measurements on powdered coal. Such measurements were completed successfully last year, but we question the compositions of the specimens, which were prepared off-site. The results from the compression probe thermal conductivity apparatus will be compared with linear hot-wire measurements on powdered and chunk coal.

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

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

Work on gas hydrates has continued. Enthalpic heat capacity measurements have been completed on pure and mixed tetrahydrofuran hydrates. Ethylene oxide hydrates have been prepared and conditioned. A chamber that will permit thermal conductivity measurements at elevated pressures has been designed and fabricated. The thermal expansion measurement system has been modified to permit measurements on hydrates.

A draft of a summary report on oil shale research needs has been completed. Research plans for shales have been formulated, and a preproposal for shale research has been developed.

External funding is being sought for the application of some of our measurement techniques (for coal) to practical problems associated with coal gasification.

Development of SRM's

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

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

Research for the development of high-temperature insulation SRM's is funded by DoE. These SRM's will fill an existing gap in the range of available thermal conductivity SRM's and are of interest to researchers and manufacturers in the chemical and related industries.

Biphenyl (SRM 2223) and mercury (SRM 2224) have been certified as temperature and enthalpy-of-transition standards according to procedures outlined in NBS Special Publication 260-99. The certification program will continue with certification of standards for the ambient and high temperature regions. The heat capacity of 9-methylcarbazole has been measured by adiabatic calorimetry from 6 to 345 K and by differential scanning calorimetry (DSC) from 125 to 350 K. The final comparisons of these results to determine whether heat capacity standards can be developed by scanning calorimetry will be completed shortly. A study of the energy calibration of DSC's, as a function of temperature and enthalpy, is also in progress.

Cryocooler Studies

R. Radebaugh, P. Bradley, J. O'Keefe, V. Arp, J. Gary*

A pulse tube refrigerator was built under a NASA-Ames contract and reached a record low temperature of 60 K in one stage. The lowest temperature previously reached with a pulse tube refrigerator was 105 K by a group from Moscow Technical High School. This new work has led to the device becoming a serious alternative to other refrigeration schemes that have more moving parts. The pulse tube refrigerator has only one moving part. A test apparatus to measure the efficiency and refrigeration power per unit mass flow has been constructed under the same program. Measurements of efficiency and refrigeration power have been made on four different pulse tubes. The results show intrinsic cooling efficiencies as high as 50 to 90 percent of Carnot in some cases and large refrigeration powers. These results are published in an NBS Technical Note and a paper presented at the Fourth International Cryocooler Conference in September 1986.

Under a five-year Air Force (AF) contract, the regenerator test apparatus was modified to make tests in the presence of pressure waves to simulate the environment seen by regenerators in an actual refrigerator. A high specific-heat material, GdRh, has been formed into powder for testing as a regenerator. This material was sent to an AF contractor for tests in an actual refrigerator. It increased the refrigeration power by 23 percent and decreased the low temperature limit from 7.1 K to 6.2 K. This material is now being tested in the NBS apparatus. Theoretical and experimental studies of the effect of the phase angle between compressor and expander pistons on regenerator performance are in progress and indicate overall refrigerator improvements can be made by a proper choice of phase angle. A computer program for the first step, optimization of regenerators, has been developed and the floppy disk for use on a personal computer is available upon request to the Air Force.

The least reliable component of present cryocoolers is the mechanical compressor. A proposed alternative uses a thermal compressor in which the gas to be compressed is first adsorbed on charcoal at a low pressure. The charcoal is then heated slightly and the adsorbed gas is driven off at some higher pressure. Only slow-moving check valves are needed to provide continuous flow in one direction. The necessary data to design a helium-charcoal compressor is lacking, but a program funded by the Air Force Space Technology Center has allowed us to measure the adsorption characteristics of helium on charcoal in the temperature range 10 to 77 K. These results will be published in the journal Cryogenics. Measurements on other charcoals as well as measurements of heats of adsorption are in progress.

Refrigeration reliability can be improved by the use of redundant cryocoolers. That approach requires the use of heat switches between the cryocoolers and the sensor to be cooled. One technique uses pressure contact between two metals. Required forces are about 13 000 N (3 000 lb). No data existed on the thermal conductance of such contacts at cryogenic temperatures. With funding from the Air Force Space Technology Center, we have made measurements on three pairs of metal samples, at temperatures from 10 K to room temperature and forces from 45 N (10 lb) to 27 000 N (6 000 lb). The data have been used by an AF contractor for the design of heat switches.

*NBS Center for Applied Mathematics

Metal Combustion in High Pressure Oxygen

J.W. Bransford, J.A. Hurley, I. Vazquez, P.I. Billiard

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

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

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

Thermal Properties of Advanced High-Temperature Materials

L.L. Sparks

Ceramics and ceramic based composites continue to develop as replacements for metals and plastics in electronic components and high performance engines and structures. Research on these materials has traditionally been in the areas of processing and mechanical properties. Thermal properties must be known for advanced applications now being contemplated or, in some cases, actually incorporated in working designs. The properties in question include thermal conductivity, thermal expansion, heat capacity, and thermal diffusivity. Knowledge of these properties is required to allow ceramics to be used in applications such as unlubricated bearings, high-temperature reactors, turbine rotors, adiabatic diesel engines, turbo compressors, thermal barriers, electrical components, and substrates for electronic components.

Three projects to address these needs are active within the group: (1) continued development of a steady-state thermal conductivity apparatus to allow ceramics and ceramic composites to be studied to 1270 K; (2) completion of a guarded-hot-plate thermal conductivity apparatus to allow ceramic fiber insulation to be studied to 800 K; and (3) alteration of the existing optical dilatometer to study foamed ceramics at low temperatures.

A third thermal conductivity apparatus is required to satisfy very high temperature (2300 K) thermal conductivity needs. Specifics of this system continue to be considered; a transient technique will probably be chosen. Development of this system will follow proof testing of the steady state system. Currently available apparatuses to study thermal expansion and heat capacity will be renovated as required to allow use at high temperatures.

Oxidation of Metals in High Pressure and High Temperature Oxygen

J.W. Bransford, J.A. Hurley

A thermogravimetric apparatus has been designed. The apparatus will be used to directly determine the oxidation rate of important technical alloys in high temperature and high pressure oxygen. The data generated by these studies will be of interest to all users of oxygen at high temperature and elevated pressure.

5. HONORS AND AWARDS

None.

6. PUBLICATIONS

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Giarratano, P.J., Arp, V.D. and Kumakawa, A., Limits to optical measurement of heat transfer in high-gradient systems, to be published in Applied Optics.

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Jin, M.F., Michel, F.C. and Noble, R.D., Kinetics of copper extraction using (anti-2-hydroxy-5-nonylbenzophenone oxime), to be published in Polyhedron.

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7. TALKS

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Giarratano, P.J., Experimental Studies of Transient Heat Transfer and Measurement of Thermophysical Properties at High Temperature and in Low Gravity, University of Colorado, Boulder, CO, Apr. 9, 1986.

Giarratano, P.J., Experimental Studies of Transient Heat Transfer and Measurement of Thermophysical Properties at High Temperature and in Low Gravity, Electro Technical Lab., Tsukuba, Japan, July 31, 1986.

Giarratano, P.J., Experimental Studies of Transient Heat Transfer and Measurement of Thermophysical Properties at High Temperature and in Low Gravity, Kyushu University, Fukuoka, Japan, Aug. 6, 1986.

Giarratano, P.J., Experimental Studies of Transient Heat Transfer and Measurement of Thermophysical Properties at High Temperature and in Low Gravity, Hitachi Corp., Kudamatsu, Japan, Aug. 7, 1986.

Giarratano, P.J., Experimental Studies of Transient Heat Transfer and Measurement of Thermophysical Properties at High Temperature and in Low Gravity, Osaka University, Osaka, Japan, Aug. 9, 1986.

Hurley, J.A., Oxidation Studies on Metallic Alloys using Differential Thermal Analysis, American Chemical Society, Eighth Rocky Mountain Regional Meeting, Denver, CO, June 9, 1986.

Hust, J.G., Specific Heat of Insulations, ASTM C16.30 Forum on Reference Materials, Louisville, KY, Mar. 12, 1986.

McDermott, K.M., Differential Thermal Analysis Studies of the Effects of Heat Treatment on Transitions in Hafnium-Bearing Superalloys, American Chemical Society, Eighth Rocky Mountain Regional Meeting, Denver, CO, June 9, 1986.

Noble, R.D., Facilitated Transport of Gases, International Membrane Conference, Tubingen, West Germany, Sept. 5, 1986.

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Perkins, R.A., Separation of Proteins/Enzymes by Aqueous Two Phase Partition, American Chemical Society, First International Conference on Separation Science and Technology, New York, NY, Apr. 16, 1986.

Powers, L.A., A Method for the Prediction of Equilibrium Values in Practical Solvent Extraction Systems (Application to Ammoniacal-copper Systems) International Solvent Extraction Conference, Munich, West Germany, Sep. 12, 1986.

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Slaff, G.F., Problems (and Solutions?) in Bioseparations, Lehigh University, Bethlehem, PA, May 27, 1986.

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Way, J.D., Facilitated Transport of Acid Gases in Ion Exchange Membranes, Dow Chemical Company, Central Research, Walnut Creek, CA, Mar. 3, 1986.

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Way, J.D., Facilitated Transport of Acid Gases in Ion Exchange Membranes, Separation and Purification, Gordon Conference, New London, NH, Aug. 14, 1986.

Way, J.D., Facilitated Transport of Acid Gases in Ion Exchange Membranes, Air Products and Chemicals, Allentown, PA, Sep. 26, 1986.

Welch, J.F., Propagation of Error in the Analysis of Performance of an Incinerator, Kansas State University, Manhattan, KS, May 21, 1986.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

J.W. Bransford

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

Chemical Engineering Science Division Hazards Review Committee (Member)

J.A. Brennan

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

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

J.E. Callanan

Calorimetry Conference Board of Directors (Director)

Calorimetry Conference Standards Committee (Member)

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

American Chemical Society, Fuel Division (Membership Chairman)

American Chemical Society, 1986 Regional Meeting (Symposium Co-chairman)

NBS Boulder Laboratories Editorial Review Board (Member)

M.J. Hiza

American Institute of Chemical Engineers, National Cryogenics Committee 13h (Member)

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

J. Hord

American Institute of Chemical Engineers, Research Committee (Second Vice Chairman and Chairman of Oversight Subcommittee)

J.G. Hust

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

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

International Thermal Conductivity Conference (Vice Chairman of Governing Board)

K.M. McDermott

Rocky Mountain Thermal Analysis Forum (Board Member)

R.D. Noble

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

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

R. Radebaugh

Federal Government Interagency Panel on Refrigeration (Member)

Cryogenic Engineering Conference Board (Chairman)

Conference on Cryocoolers--1986 (Program Committee)

V.N. Schrodt

American Institute of Chemical Engineers, National Program Committee (Chairman)

Industrial and Professional Advisory Council, Department of Chemical Engineering, The Pennsylvania State University (Chairman)

S.K. Sikdar

AAAS, Physical Sciences Division, Graduate Student Speech Contest (Judge, Boulder, CO, Apr. 1986)

University of Colorado Biotechnology Advisory Council, Department of Chemical Engineering (Member)

ASTM Committee on Membrane Characterization for Biotechnology (Chairman)

American Chemical Society, Separation Science and Technology Subdivision, Program Committee (Member)

L.L. Sparks

ASTM E20 Committee on Temperature Measurement, Thermocouples Subcommittee (Member)

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

ASTM C9 Committee on Concrete and Concrete Aggregates (Member)

R.O. Voth

Chemical Engineering Science Division Hazards Review Committee (Chairman)

J.F. Welch

ASTM D34 Committee on Waste Disposal (Member)

ASTM D34.08 Subcommittee on Thermal Treatment (Acting Secretary)

ASTM D34.08.06 Task Group on Calculational Methods (Chairman)

EDITORSHIPS

M.J. Hiza

Fluid Phase Equilibria (Editorial Board)

Proceedings of the 6th Cryogenics Intersociety Symposium, American Institute of Chemical Engineers Symposium Series, October 1986. (Co-editor with A.J. Kidnay)

J.G. Hust

Journal of Thermal Insulation (Editorial Board)

R.D. Noble

Proceedings of the Membrane Separation Technology Symposia, American Chemical Society Symposium Series, June 1986. (Co-editor with J.D. Way)

S.K. Sikdar

Gas Separation and Purification, Butterworth (Member of International Editorial Board)

J.D. Way

Proceedings of the Membrane Separation Technology Symposia, American Chemical Society Symposium Series, June 1986. (Co-editor with R.D. Noble)

9. PROFESSIONAL INTERACTIONS

FACULTY APPOINTMENTS

J.E. Callanan

Adjunct Associate Professor, Department of Chemistry, University of Colorado

M.C. Jones

Adjunct Associate Professor, Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines

R.D. Noble

Adjunct Associate Professor, Department of Chemical Engineering, University of Colorado

INDUSTRY

M.J. Hiza

Collaboration with T. Selover, SOHIO, Cleveland, OH, on data for the petrochemical industry and activities of the CODATA Task Group--Data for the Chemical Industry.

Collaboration with C.F. Spencer, M.W. Kellogg, Houston, TX, on CODATA activities--Data for the Chemical Industry.

Collaboration with M.E. Baltatu, Fluor Engineering Inc., Irvine, CA, on activities of the CODATA Task Group--Data for the Chemical Industry, specifically in the area of biotechnology.

S.E. McManus

Collaborative research with C. Griffis and K. Kothari, Gas Research Institute, Chicago, IL, on the effects of flow disturbances and installation design on flow meters.

R. Radebaugh

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

Cooperative research with C. King, Alabama Cryogenic Engineering, Huntsville, AL, on pulse tube refrigeration.

Cooperative research with G. York, Hughes Aircraft, El Segundo, CA, on thermal conductance of metal pressure joints.

J.D. Siegwarth

Collaborative research with Joel Blumenthal, Micromotion, Inc., Boulder, CO, supplied densimeter to Micromotion for fluid density calibration.

L.L. Sparks

Coauthorship of paper with R.W. Rosser, Hughes Aircraft, Culver City, CA, on thermal behavior of polymer composites.

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.

Collaboration and proposal preparation with D.R. Kassoy, University of Colorado, Boulder, CO, on thermo-acoustic convection.

B.R. Bateman

Cooperative research with R.B. Owen, NASA-MSFC, Huntsville, AL, concerning use of double exposure holography and other optical methods to measure the density gradient of protein solutions in a capillary.

Cooperative research with A.D. Randolph, University of Arizona, Tucson, AZ, on crystallization of biomolecules in space.

Cooperative research with S. Selim, Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, Golden, CO, on measurement of diffusion coefficients of proteins.

Collaborative research with J.R. Whetstone, NBS/CCE, Gaithersburg, MD, and J.L. Savidge, School of Chemical Engineering and Materials Science, University of Oklahoma, Norman, OK, on calculating critical flow factors for sonic nozzles using an equation of state for natural gas.

S.D. Bischke

Collaborative research with P. Glugla, Department of Chemical Engineering, University of Colorado, Boulder, CO, on amino acid transport through ionomeric membranes.

J.E. Callanan

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

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

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

Collaborative research with D.F. Vecchia, NBS Center for Applied Mathematics, Boulder, CO, on statistics of instrument calibration.

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

D.E. Daney

Cooperative research with G. Mattingly, NBS/CCE, Gaithersburg, MD, on modeling of fluid tangential vortex motion in cylindrical tanks near zero-g for mechanically induced transfer between tanks.

P.J. Giarratano

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

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

M.J. Hiza

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

Collaboration with G. Mattingly, NBS/CCE, Gaithersburg, MD, on experimental measurement needs for fluid management in microgravity environments.

J.G. Hust

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

Collaborative research with T. Faison and B. Rennex, NBS Center for Building Technology, Gaithersburg, MD, on thermal insulation standard reference materials.

M.C. Jones

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

Collaborative research with R.B. Owen, NASA-MSFC, Huntsville, AL, on application of optical techniques to heat and mass transfer problems.

B. Louie

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

P.R. Ludtke

Cooperative research with A.D. McInturff, Fermilab, Batavia, IL, on pumping of superfluid liquid helium with special pump.

K.M. McDermott

Collaborative research with D. Vecchia, NBS Center for Applied Mathematics, Boulder, CO, on standard reference materials development.

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

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

R.D. Noble

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

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

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

R.A. Perkins

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

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

Collaborative research with H. Cabezas, Department of Chemical Engineering, University of Arizona, Tucson, AZ, on statistical mechanics of aqueous protein and polymer solutions.

Collaborative research with J.B. Joshi and S.B. Sawant, Department of Chemical Technology, University of Bombay, Bombay, India, on aqueous two-phase separation of proteins.

L.A. Powers

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

R. Radebaugh

Cooperative research with P. Storch and K. Timmerhaus, Department of Chemical Engineering, University of Colorado, Boulder, CO, on pulse tube refrigeration.

S.K. Sikdar

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

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

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

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

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

Collaborative research with H. Cabezas, University of Arizona, Tucson, AZ, on the modeling of protein partition in two-phase aqueous systems.

Collaborative research with J.B. Joshi and S.B. Sawant, University of Bombay, Bombay, India, on the mass transfer of proteins in two-phase systems.

C. Sindt

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

Cooperative research with G. Mattingly, NBS/CCE, Gaithersburg, MD, on acquisition and analysis of orifice meter data for water in the NBS water flow measurement facility at NBS, Gaithersburg, MD.

L.L. Sparks

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

J.D. Way

Cooperative research with C.A. Koval, Department of Chemistry, University of Colorado, Boulder, CO, on facilitated transport of gases and liquid phase hydrocarbons.

J.F. Welch

Collaboration with J. Elias and R. Lundy, Fermi National Accelerator Laboratory, Batavia, IL, on safety analysis.

Collaboration with M. Roberts, Naval Civil Engineering Laboratory, Port Hueneme, CA, relative to application of supercritical technology to treatment of Navy hazardous wastes.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

A Symposium on Thermal Analysis in the Characterization of Material Behavior at the American Chemical Society Rocky Mountain Regional Meeting in Denver, CO, June 9-13, 1986 was organized and chaired by J.E. Callanan and A.R. Greenberg (University of Colorado, Boulder, CO).

Membranes: Theory and Applications, four sessions held at the American Chemical Society Rocky Mountain Regional Meeting in Denver, CO, June 11-12, 1986. J.D. Way and R.D. Noble, session chairmen.

Session [59], A Panel Discussion and Open Forum on Measurement Needs in the Chemical and Related Industries, held at the American Institute of Chemical Engineers Summer National Meeting in Boston, MA, Aug. 26, 1986. J. Hord, session chairman.

Fourth International Cryocooler Conference, held at Easton, MD, Sep. 25-26, 1986. Ray Radebaugh, member of program committee.

Sixth Cryogenics Intersociety Symposium of the American Institute of Chemical Engineers, ASME, and IIR, held in conjunction with the 1986 Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, FL, Nov. 2-7, 1986. M.J. Hiza, member of organizing committee and co-editor of symposium proceedings.

Session [7], Safety and Reliability of Cryogenic Systems, held at the 1986 Annual Meeting of the American Institute of Chemical Engineers, Miami Beach, FL, Nov. 5, 1986. J. Hord, session vice-chairman.

WORKSHOPS

None.

SEMINARS

Ms. Sharon Hines, Raptor Education Foundation, Denver, CO: Introduction to Raptors, Birds of Prey, Nov. 1, 1985.

Mr. Bill Herbert, Coors Porcelain Company, Golden, CO: A Little Giant in a Big Shadow, An Overview of the Coors Porcelain Company, Nov. 22, 1985.

Dr. Alan S. Michaels, Alan Sherman Michaels, Inc. Boston, MA: Membrane Processes for Bioproduct Recovery, Jan. 6, 1986.

Dr. Fred Fickett, NBS Center for Electronics and Electrical Engineering, Boulder, CO: Fusion Energy Research, Current Status, Jan. 31, 1986.

Dr. Dave Clough, Department of Chemical Engineering, University of Colorado, Boulder, CO: Chemical Process Control--A 20-Year Perspective, Feb. 28, 1986.

Mr. Tarun K. Ghose, Department of Chemical Engineering, University of Delaware, Newark, DE: Advances in Immobilized Cell Technology, Mar. 21, 1986.

Dr. Lawrence L. Tavlarides, Department of Chemical Engineering and Materials Science, Syracuse University, Syracuse, NY: Modeling and Scale Up of Reactors for Liquid-Liquid Dispersions Undergoing Reaction, Apr. 1, 1986.

Dr. Arthur E. Humphrey, Lehigh University, Bethlehem, PA: Monitoring Biochemical Systems, Apr. 2, 1986.

Dr. Quen Shen Shu, Fermi National Accelerator Laboratory, Batavia, IL: A Study to Reduce Heat Flux through Multilayer Insulation and Support Structures in Large Scale Superconducting Magnets, Apr. 15, 1986.

Dr. M.M. Sharma, Department of Chemical Technology, Matunga, Bombay, India: Separations through Reactions, May 1, 1986.

Dr. E. Freire, University of Tennessee, Knoxville, TN: Thermodynamics of Insertion and Structural Stability of Membrane Proteins, June 10, 1986.

Mr. M.P. Thien, Massachusetts Institute of Technology, Cambridge, MA: Separation and Concentration of Amino Acids Using Liquid Emulsion Membranes, June 13, 1986.

Mr. Thomas J. Chresand, Colorado State University, Fort Collins, CO: Substrate Diffusivities in Cell-Collagen Matrices, July 7, 1986.

Dr. V.F. Baston, Physical Sciences, Inc., Middletown, PA: Three Mile Island (TMI-2), A Chronological Review, July 11, 1986.

Dr. David W. Woodruff, General Electric Co., Schenectady, NY: Chemical Engineering in the World of Microelectronics, Aug. 4, 1986.

Dr. D. Chatterji, The BOC Group R&D Center, Murray Hill, NJ: Business and Technical Interests of the British Oxygen Company Group, Aug. 22, 1986.

Mr. Mike Prairie, California Institute of Technology, Pasadena, CA, Experimental and Modeling Investigations of Steady-State and Dynamic Characteristics of Ethylene Hydrogenation on Alumina Supported Pt, Sep. 29, 1986.

TECHNICAL ACTIVITIES
OF THE
THERMOPHYSICS DIVISION

N. A. Olien, Chief

1. INTRODUCTION

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

The approach is to conduct research on fundamental theoretical models, new concepts and phenomena, and predictive algorithms in synergism with experimental programs. The experimental research is aimed at developing new measurement techniques and providing highly accurate data for the properties of carefully selected pure fluids and mixtures, as well as high temperature solids, which are representative of broad classes of fluids and materials encountered in many industries. An essential ingredient of the above efforts will be the critical evaluation and correlation of data leading to the publication of Standard Reference Data.

All industrial processes and certainly those in the chemical and fuel industries are steadily moving toward alternative and more complex base feedstocks, which in turn yield more complex, and often corrosive and hazardous, conversion products and often involve higher temperature processes. A very significant factor in the application of the research described here is the widespread use of process simulation and computer-aided design in the development, optimization, and control of processes and plants in the chemical, fuel, and related industries. Key ingredients of all process simulators are the data and models for the properties of fluids and other materials encountered in the processes. Major outputs of the research program described here are property data in the form of predictive theoretical models and correlations, which can be readily incorporated into process simulator and process control algorithms.

Thermophysics Division research addresses scientific issues of national importance for which NBS expertise, and its impartial position, are critical to data acceptance and to the resolution of problems of equity in trade for such products as ethylene, natural gas, steam, carbon dioxide, etc. The majority of the work is directed toward problems of the future. These include, but are not restricted to, the following: 1) fluids encountered in the conversion and utilization of coal, oil shale, heavy oils, and tar sands to gaseous and liquid feedstocks and fuels which, in turn, contain substantial amounts of aromatic organics and associating compounds (N, O, S); 2) fluid mixtures encountered in bioprocess engineering, which are essentially aqueous solutions containing macromolecules; and 3) high temperature solid and fluid property needs of government agencies for energy, defense, and aerospace (e.g. DoE, DoD, NASA), where NBS expertise can provide specific results. The strategy is to perform basic research, generic to the science underlying the chemical, fuel, power, and aerospace industries, which requires the special role of NBS as an impartial national laboratory excelling in experimental and theoretical results and their interpretation.

2. GOAL

The goal of the Division is to provide standard measurement procedures, benchmark experimental data, and reliable methods of predicting key thermophysical properties of high temperature solids and industrially important chemicals, fuels, and related fluids. These data are used: in the innovation, design, and control of chemical processes; to insure equity in domestic and international exchange of products; and by NBS and others as benchmark data to extend versatile computational techniques which reliably predict the properties of broad classes of substances over extended operating ranges.

The output of this program assists the chemical, fuel, power, aerospace, and related industries in maintaining and enhancing their competitiveness in the international marketplace and in making their processes more efficient and able to accept a broader array of input feedstocks, and in providing avenues to the development of new products.

3. GROUP AND PROGRAM FUNCTIONS

GROUPS

° Equation of State and Statistical Physics (Gaithersburg, MD) - J. M. H. Levelt Sengers, Group Leader

The Group conducts fundamental experimental and theoretical studies of the properties and behavior of pure fluids, mixtures, and solids. Experimental activities include the development of state-of-the-art measurement techniques, benchmark data for thermodynamic properties, studies of interfacial phenomena and properties, and studies of fundamental constants. Theoretical studies include condensed matter in equilibrium and nonequilibrium, interfacial phenomena, fundamental models of the critical region, polydisperse fluid mixtures, aqueous and polymer solution thermodynamics, and thermophysical properties of solids by a variety of analytical techniques and by computer simulations. Major non-CCE sponsors of the work of this Group include the DoE, NASA, and the NBS Office of Standard Reference Data (OSRD).

° Properties of Fluids (Boulder, CO) - W. M. Haynes, Group Leader

This Group has a research program which integrates experimental measurements, theoretical studies, and critical evaluation of data, all designed to lead to a basic understanding of fluid behavior. Outputs are data and theoretically-based predictive models for the properties of technically important complex mixtures and pure fluids. The fluids of interest include common inorganics, industrial chemicals, hydrocarbons, coal conversion products, heavy oils, biochemical solutions, etc. Principal non-CCE sponsors of the work of this Group include the DoE, the Gas Research Institute, the DoD, industrial consortia, and the OSRD.

PROGRAMS

° Dynamic Measurements (Gaithersburg, MD) - A. Cezairliyan, Project Leader

This program develops dynamic (millisecond and microsecond) measurement techniques and performs measurements of selected thermophysical properties of high temperature materials over the range 1500 - 10 000 K. Materials investigated include high temperature conductors, refractory materials, metallic composites, and high temperature Standard Reference Materials. The unique capabilities of this laboratory provide the means to perform accurate measurements in temperature regimes and at high heating rates where conventional techniques fail. Work on this program is largely supported by NASA and the DoD.

° Complex Fluids (Boulder, CO) - H. J. M. Hanley, Project Leader

This program provides advanced theoretical and experimental techniques for the study of the behavior of complex fluid mixtures. It is totally integrated with the technical activities of the Properties of Fluids Group.

4. SELECTED PROJECT SUMMARIES

The organizational realignment of October 1985, which brought the Properties of Fluids Group in Boulder into the Thermophysics Division, completed the integration of thermophysical property research within the National Bureau of Standards. The Dynamic Measurements Program and the Complex Fluids Program are attached to the Division Office, while the remainder of the research of the Division is now organized into two groups, one in Gaithersburg and one in Boulder. Although each Group possesses certain areas of expertise and interest, the technical work is carried out in a manner which minimizes geographic limitations and distinctions. The reporting of the Technical Activities in this section reflects the integrated efforts of the two groups. The technical activities are described in six research areas: Equilibrium Properties of Fluids and Fluid Mixtures; Behavior of Complex Fluids; Properties of Supercritical Fluid Mixtures; Interfacial Properties and Behavior; Transport Properties of Fluids and Fluid Mixtures; and Thermophysical Measurements by Dynamic Methods.

Equilibrium Properties of Fluids and Fluid Mixtures

A substantial part of the research effort of the Thermophysics Division, both experimental and theoretical, is devoted to studies of the equilibrium properties of pure fluids and mixtures. Since so much of our mixture work involves corresponding states and the mapping of mixture surfaces onto pure fluid surfaces, pure fluid work is usually undertaken to provide basic data for the development of mixture models. Clearly this area of our research is one which has close ties to our outside users and represents a traditional NBS role in providing data for industrial and engineering applications.

J.F. Ely and M.L. Huber are engaged in the development of advanced corresponding states theories which incorporate both microscopic theory and pure fluid corresponding states approaches. Included is work on the hard sphere expansion theory and its underlying mean density approximation. The advantage of this approach is that theoretical advances can be directly incorporated into the models. A major goal of this work is the development of models which provide for polar-nonpolar interactions. In conjunction with this goal, a computer model for carbon dioxide-rich mixtures (DDMIX) has been developed and will be distributed by OSRD. Dr. Ely and D.G. Friend are applying the Wagner equation of state to light hydrocarbons with excellent results, especially in the extended critical region. Ely is also completing the development of an advanced version of his TRAPP computer code which will provide predicted data in the two phase region. Work is also progressing on the application of the TRAPP model to other classes of molecules such as refrigerants. G. Morrison (with D.A. Didion and M.O. McLinden of the NBS Center for Building Technology) is engaged in a long term collaborative effort to improve the operating efficiency of heat pumps and refrigeration systems, particularly systems using mixed refrigerants. The work involves both experimental research and equation of state development, and includes extensive phase equilibria studies. The latter efforts include a substantial amount of interaction with energy and refrigeration companies. A report summarizing much of this collaborative work was published this past year.

As stated earlier, a traditional role for NBS is the provision of Standard Reference Data for industrial, academic, and government use. During the past year, B.A. Younglove and J.F. Ely completed the second volume of an OSRD series of thermodynamic data books; this one covers the lower alkanes. The results of both books are incorporated in the computer code MIPROPS, developed by R.D. McCarty and distributed by OSRD in both mainframe and personal computer (PC) versions. R.D. Goodwin has completed critical evaluations of thermodynamic data for methanol and benzene and is currently working on toluene. Computer packages such as TRAPP, DDMIX, and MIPROPS are examples of the format in which much of our research will ultimately appear. The ubiquitous nature of the personal computer dictates that our computer results must eventually be PC compatible, even though some numerical precision is sacrificed in the process. R.D. McCarty has extensive experience with corresponding states applications, including propellent data for NASA. With R.T. Jacobsen of the University of Idaho and J.M.H. Levelt Sengers, J.V. Sengers, and colleagues at the University of Maryland, he has completed work on the final formulation for ethylene for OSRD which will be published by IUPAC. McCarty and Jacobsen are also engaged in the development of a highly accurate equation of state for air in support of the National Aerospace-plane Project. A related project aimed at the development of models for fluid mixtures involves J.C. Rainwater and M.R. Moldover. Their model is applicable to liquid-vapor equilibria for a wide range of mixtures in the critical and extended critical region. The model provides an excellent correlating technique for mixtures ranging from hydrocarbons to air, including some polar fluids.

During the past four years, the Thermophysics Division has greatly expanded its experimental capability in several areas including equilibrium, transport, and interfacial measurements. J.M.H. Levelt Sengers, D. Linsky, and H.A. Davis have completed the development of an automated Burnett PVT apparatus which includes a unique pressure controlling system. G. Morrison, L.A. Weber, F. Guzman, and H.A. Davis completed work on a variable volume VLE apparatus. Both of these apparatuses are now in routine operation. During the next year W.M. Haynes expects to complete work on an automated balance densimeter. A guest worker, R. Masui, from the Japan National Laboratory for Metrology will work with Dr. Haynes. The balance densimeter has been moved from Gaithersburg to Boulder for the completion of its development. The initial work on the apparatus was done by Dr. Masui working with J.M.H. Levelt Sengers and R.F. Chang. This apparatus, along with Dr. Haynes' low temperature magnetic suspension densimeter will provide the Division with unprecedented capability for high accuracy PVT and PVTx measurements in the range 90 - 500 K. Of great importance to our experimental work is the equipment and expertise existing in the Division for the gravimetric preparation of highly characterized fluid mixtures. The importance of this capability, coupled with the existence of an advanced analytical laboratory, cannot be overemphasized.

From the standpoint of measurement programs in equilibrium properties, the Thermophysics Division has completed a substantial body of important research in recent months. G.C. Straty completed PVT measurements on benzene and toluene to 723 K and 673 K, respectively. In both cases measurements extended beyond the point at which thermal decomposition became significant. The techniques developed for analyzing and reporting data such as these are discussed in the complex fluids section below. D. Linsky completed PVT measurements on the isobutane - isopentane system, mixtures used as geothermal working fluids; the results extend to 430 K. These experimental data were correlated by an equation of state developed by J.S. Gallagher. This marks the completion of a major experimental and theoretical project in support of the Heber Geothermal Power Plant. T.J. Bruno has performed fugacity measurements on a series of hydrogen binary mixtures (with ethane, carbon dioxide, and carbon monoxide) using a unique apparatus which employs a palladium membrane. L.A. Weber has completed VLE measurements on a series of mixtures of hydrocarbons with refrigerants. Related PVT measurements on pure refrigerant 13 have been completed by J.W. Magee, using an isochoric PVT apparatus, recently automated and upgraded by him. Dr. Magee will be performing additional PVT measurements on carbon dioxide-hydrocarbon systems in support of the supercritical consortium project discussed below. Dr. Magee, with J.E. Mayrath, is conducting measurements of the specific heat at constant volume on a series of methane-ethane mixtures.

The Thermophysics Division is one of the few laboratories in the world with the capability of measuring sound speed in fluids. M.R. Moldover (with J. Mehl of Delaware University) has developed the spherical acoustic resonator technique to the point that measurements of unprecedented accuracy and precision are possible. Four laboratories around the world have built apparatus based upon Dr. Moldover's ideas. During this past year, Dr. Moldover (with J.M. Trusler of University College, London) completed sound speed measurements in gaseous argon which should yield a new value for the universal gas constant R, with an uncertainty of 5-10 parts per million (a five-fold improvement). In addition to fundamental constant work, the acoustic resonator technique has application in more routine measurements, where it offers the advantages of high accuracy and rapid data taking. Dr. Moldover has worked in Boulder with B.A. Younglove and N.V. Frederick in applying the technique to sound speed measurements in gaseous mixtures. The natural gas industry is very interested in using sonic nozzles as secondary flow measurement standards, but has been hampered by the lack of accurate data upon which to base performance. There are no experimental data in the literature for sound speed in gas mixtures other than air. We expect the spherical resonator apparatus to become operational soon. In the meantime, Dr. Younglove has conducted sound speed measurements using a cylindrical resonator of his own design. Thus far he has completed measurements on a series of mixtures of methane with ethane and nitrogen. These results represent the first high accuracy results ever obtained for gas mixtures. In a complementary effort, R.D. McCarty is developing a highly accurate predictive model for sound speed in natural gas and similar mixtures.

Behavior of Complex Fluids

The research of the Thermophysics Division is moving in the direction of developing the experimental techniques to study more complex mixtures and theoretical methods for modeling the behavior and properties of ever more complex mixtures. We have started to address issues involving the thermophysical properties of biological fluid mixtures. Although we have not actually begun work in this area, we are organizing a one-day workshop at NBS-Gaithersburg in March 1987 which will address the needs for property research in this area and the experimental and theoretical priorities associated with thermodynamics in biotechnology. Our current research in complex fluids certainly makes this a logical next step in our progression toward complexity.

H.J.M. Hanley and G.C. Straty are investigating universal behavior in liquids, i.e. behavior that depends only weakly on the specific nature of the molecule. The studies are geared to emphasize trends and similarities between simple and complex molecules by studying relatively simple molecules like supercooled glycerol which displays complex behavior such as shear dependent thermodynamics. The research involves considerable computer simulation work (including collaborations with D.J. Evans and others at Australian National University, Oak Ridge, and Institut Laue-Langevin). J.F. Ely, J.C. Rainwater, and D.G. Friend are also involved in this theoretical work. On the experimental side, considerable beam time has been obtained over the past year on the NBS small angle neutron scattering (SANS) facility using glycerol in equilibrium. A shearing cell for the SANS facility is under development and we expect results from that work in the next year.

In addition to the above work that involves molecular dynamics calculations (MD) on the new NBS supercomputer, R.D. Mountain is engaged in extensive MD studies in condensed matter physics with emphasis on phase transitions and metastability. With F.E. Sullivan of the NBS Center for Applied Mathematics and G.W. Mulholland of the NBS Center for Fire Research, Dr. Mountain is studying the kinetics of the growth of particulates undergoing Brownian motion and aggregation by means of computer simulation using a "Brownian dynamics" technique. Results have been obtained for the free molecular regime and for the continuum limit for the background gas. The scattering of light by these aggregates is also being examined. In the course of the work, a very efficient simulation code for the NBS supercomputer was developed. Dr. Mountain is also using MD to investigate the dynamical processes involved in the phenomenon of collision-induced absorption of far infrared radiation in rare gas mixtures. Other MD work includes a study of molecular size effects in model gas mixtures by J.F. Ely, Monte Carlo simulations of multicomponent lattice Lennard-Jones mixtures by J.R. Fox, and MD studies of phase transitions in model polar fluids by J.B. Hubbard. It is interesting to note at this time that the supercomputer has become an indispensible tool in the work of the Thermophysics Division. During Fiscal Year 1986, the Thermophysics Division accounted for nearly 40% of the total central-processor time on the NBS supercomputer.

An important area of research for the Thermophysics Division is aqueous solutions. The Division has a history of work on the properties of water and steam with involvement from L. Haar, J.M.H. Levelt Sengers, J.S. Gallagher, and J.V. Sengers. J.B. Hubbard has also done extensive work on nonequilibrium theories of electrolyte solutions. The latter includes a series of lectures on the subject by Dr. Hubbard at a NATO Advanced Study Institute this past summer. J.M.H. Levelt Sengers chairs Working Group A of the International Association for the Properties of Steam (IAPS) and co-organized a workshop on aqueous solutions at the IAPS meeting in Dusseldorf in September. Dr. J.V. Sengers, with a number of co-workers, has been engaged in the comprehensive study of the thermodynamic and transport properties of ordinary and heavy water for IAPS. The work on aqueous solutions is expanding, not only because of its inherent importance, but also because research on aqueous solutions will play a large part in future efforts involving the properties of biological solutions. Under the auspices of the OSRD, we have undertaken a fundamental study of the solubility of gases in water, as a function of temperature and pressure. Current plans call for the use of a perturbation technique, in order to map solution properties onto those of a pure solvent. Dr. Levelt Sengers, along with Dr. Hubbard (with collaboration from J.C. Rasaiah of the University of Maine) and J.S. Gallagher will be involved in this aspect of the effort. Molecular dynamics simulations on aqueous solutions will be carried out by R.D. Mountain.

Another area of recent work in the Thermophysics Division is the thermophysical properties of reacting fluids. Recent work by G.C. Straty involves the experimental determination of the PVT properties of methanol, benzene, and toluene at high temperatures. Liquid-vapor equilibria studies of the methanol-water system are also being performed at high temperatures by J.E. Mayrath. T.J. Bruno has completed work on an analytical facility, which provides us with extensive capability for testing and analyzing fluids prior to and during measurement programs. In conjunction with this work he has recently published an extensive compilation of data for use in chemical analysis, which will appear in 1987 as a handbook. Drs. Bruno and Straty, along with H.J.M. Hanley are preparing publications detailing protocols for characterizing reacting fluids, performing reproducible measurements on them, and reporting data from such measurements. J.B. Hubbard (with J.C. Rasaiah and S. Lee of the University of Maine and R.J. Rubin of the NBS Institute for Materials Science and Engineering) is using computer simulations to study the theory of diffusion controlled reaction kinetics in the presence of density and composition fluctuations. Dr. Bruno is working on the second generation version of a gas chromatography detector, which uses the temperature change produced when a hydrocarbon undergoes catalytic cracking as the basis for the detector.

The general area of complex fluids includes mixtures with very large numbers of constituents, and mixtures in which compositions change with temperature, pressure, and time. The Thermophysics Division is investigating the use of polydisperse fluid theory as a means of modeling these classes of complex mixtures. J.M. Kincaid, G. Morrison, and R.A. MacDonald have developed a formulation for a thermodynamic perturbation theory treatment of multicomponent and polydisperse mixtures. Phase equilibria and critical point conditions have been obtained to second order. Dr. Morrison is conducting experimental measurements of phase equilibria in model polydisperse fluids in support of this work. J.F. Ely is using a form of continuous thermodynamics in a preliminary study of water soluble polymers, with application to future research in biological fluid mixtures.

Properties of Supercritical Fluid Mixtures

The topic of supercritical fluids and the array of potential applications, ranging from enhanced oil recovery to chemical separations to biotechnology, has made the field of supercritical fluids one of large interest to the Thermophysics Division. Over and above that, however, other factors make the field even more ripe for our involvement. First of all, the Division is recognized around the world for its seminal research in the extended critical region, the critical point, and scaled equations of state. Secondly, the NBS reputation for excellence and accuracy in measurements and modeling very neatly coincides with industry's requirements in this case. In order for supercritical processes to achieve their full potential, properties of the supercritical solvent and its mixtures must be known to high levels of accuracy. As with most work in the Division, the research on supercritical fluids involves both experimental and theoretical work.

The most visible projects in the Division's supercritical work are two which grew out of a three-year program supported by a consortium of fourteen chemical and energy firms. J.F. Ely and J.W. Magee are working on carbon dioxide rich mixtures with the goal of developing a more accurate and general form of Dr. Ely's model, DDMIX, for near critical mixtures. The work includes extensive PVT measurements using the newly automated isochoric apparatus which Dr. Magee has developed for this project. In a related project, also supported by an industrial consortium, Dr. Ely is devloping global models for single phase and VLE of supercritical mixtures, with emphasis on polar compounds. With J.R. Fox, he is completing the development of a high accuracy equation of state for carbon dioxide which uses Dr. Fox's rescaling to improve derived property predictions. In a companion project, P.C. Albright and J.V. Sengers formulated a scaled, fundamental equation of state for carbon dioxide in the critical region which provides for "crossover" from nonanalytic to analytic behavior. A review on the subject of "crossover" has been prepared by Drs. Sengers and Levelt Sengers. A theoretically satisfactory solution to the "crossover" problem is of great importance to the construction of reliable thermodynamic surfaces for fluids and mixtures.

J.S. Gallagher and J.M.H. Levelt Sengers have completed work on impurity effects in the equation of state for the isobutane-isopentane system, including the extended critical region, which builds on previous work on impurity effects in ethylene. The effects are large and nonlinear in concentration near the mixture critical line. In related work, R.F. Chang developed a non-classical treatment of impurity effects, working out the power law dependence of partial molar volume, activity coefficient, and derived properties. Applications of the dilute mixture work to near-critical aqueous electrolyte solutions has been explored. J.C. Rainwater has developed a very generalized technique for accurately modeling LVE for a large class of mixtures from the critical line down to at least half the critical pressure. G.C. Nielson, working with Dr. Levelt Sengers, has modeled supercritical solubility using a doubly decorated lattice gas which maps the properties of the solution onto the pure solvent. The model has been fitted to solubility data for three systems at a number of temperatures. All of this work has an obvious relation to research on aqueous solutions and is intimately tied to that research.

E.J. Clark has started experiments on the solubility of high molecular weight polyethylene in hydrocarbon and halocarbon solvents. Three-phase systems have been observed over the range of temperatures investigated to date. Related theoretical work involves J.M.H. Levelt Sengers (with P. Meijer and I.L. Pegg of Catholic University) use of the Flory-Huggins model to predict global phase diagrams and tricriticality.

T.J. Bruno has designed, constructed, tested, and placed in operation a supercritical fluid chromatograph (SFC) specifically designed to measure diffusion coefficients at infinite dilution. The carrier is carbon dioxide and data have been obtained for the carbon dioxide-naphthalene system. During the developmental period, a number of highly useful innovations were introduced by Dr. Bruno including chromatographic vortex cooling, SFC injection from fluids adsorbed on glass, miniature contact thermometers for temperature control, etc.

Interfacial Properties and Behavior

The purposes of this program are to experimentally study surface tension near critical points; to 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; and to test the validity of proposed theories for interfacial phenomena and wetting. The ubiquitous occurrence of wetting layers has been demonstrated by research which began in the Thermophysics Division in 1980. It is generally recognized that wetting layers will be of concern in careful measurements of any thermophysical property of coexisting fluid phases. We have recently published an extensive review of the role of nonequilibrium phenomena in determining the thicknesses of the wetting layers which have been measured in certain recent experiments. We expect that wetting layers will play an important role in the behavior of fluids in porous media.

M.R. Moldover and J.W. Schmidt have measured the interfacial tension of three binary liquid mixtures near their consolute points. The mixtures were triethylamine + water, triethylamine + heavy water, and methanol + cyclohexane. The data were used to estimate the "universal amplitude ratios" which relate the interfacial tension to the specific-heat divergence and to the correlation length near critical points. The new measurements used a method (pendant drop) that had not been used near critical points before. The new measurements confirm the conflict between the experimental and theoretical amplitude ratios. The amplitude ratios for a wide variety of fluid systems, including polymer solutions, are mutually consistent and in the most favorable cases have an accuracy approaching ± 5%. Surprisingly, the experimental amplitude ratios do not agree with recent theoretical estimates from Monte Carlo simulations of the Ising Model or from calculations based on renormalization-group ideas. Nevertheless, the experimental amplitude ratios can be used for predicting the interfacial tension when the correlation length amplitude is known or when the heat capacity amplitude is known.

J.W. Schmidt and M.R. Moldover have systematically studied the transition from incomplete wetting to complete wetting at the liquid-vapor interface above mixtures of alcohols (methanol through hexanol) and a fluorocarbon (perfluoromethylcyclohexane). Above the transition temperature, fluorocarbon layers ($\approx$ 200 nm thick) spread across the liquid-vapor interface. Below the transition temperature, the excess fluorocarbon on the interface is less than one monolayer. The consolute temperatures of these mixtures are almost independent of the type of alcohol; however, the wetting temperatures decrease dramatically as heavier alcohols are used. This demonstrates that the occurrence of complete wetting in these mixtures is not associated with the proximity to the consolute point, contrary to widely held views. The wetting transition in the mixtures with isopropanol was studied in particular detail. Drs. Moldover and Schmidt established that this transition is first order, even when studied at very high resolution.

The ellipticity of the liquid-vapor interface was measured above mixtures of cyclohexane with methanol and with deuterated methanol. Upon deuteration the methanol-rich phase becomes heavier than the cyclohexane-rich phase. Below the consolute temperature, the methanol-rich phase forms at the liquid-vapor interface; however, its thickness is limited by the Rayleigh-Taylor instability.

P.C. Albright, R.F. Kayser and M.R. Moldover have been engaged in the development of a theory to model the increase in surface tension which occurs when a flat interface is confined to a small area. The calculation is relevant to supported liquid phase catalysis and to certain schemes for tertiary oil recovery. Recently the theory has been generalized to the case where the interface is in the form of a small sphere. The relevance of this generalization to nucleation problems is being investigated. An experiment to test the effects of confinement upon interfacial tension has been designed. The experiment uses an idealized geometry in which an interface is confined between parallel plates whose separation is varied in a precisely measured way in the range 1-4 μm.

R.F. Kayser is studying the relationship between wetting layers and intermolecular forces. Specifically, the studies involve the possible role of dispersion forces in the formation of wetting layers on walls above a liquid-vapor meniscus. Experimental results contradict theoretical calculations of the thickness of these layers. In an effort to resolve this obvious gap in understanding, Langmuir's theory for the role of ionic forces in the formation of wetting layers of water on glass was generalized to mixtures of polar and nonpolar liquids. Experimental tests of the theory are planned.

Dr. Fransisco Guzman, of Metropolitan University in Mexico City, spent a sabbatical year in the Thermophysics Division studying the relationship between the stability of transient foams and wetting transitions near liquid-liquid phase boundaries in several multicomponent liquid mixtures. A characteristic feature of liquid-liquid phase transitions is that, as the critical point is approached, one phase intervenes between the other and the surroundings - the walls of a container or the vapor over the liquid phases. It has been suggested that a jump in the stability of transient foams near the phase transition locus could be explained by the prewetting transition. Dr. Guzman set up an experiment to measure the height of a foam head as a function of the rate of flow of a spectator gas bubbled through the liquid phase. By changing the composition of the mixtures and by changing the temperature, the region near the phase boundary could be studied in great detail. The results showed partial wetting up to the critical point and that the stability of foams did display quite characteristic and elaborate behavior near the phase transition line. Concurrent with the foaming experiments, the thickness of surface layers was measured by using the ellipsometer constructed by J.W. Schmidt.

G. Morrison, H.A. Davis and I.L. Pegg have completed the development of a film balance. The balance is composed of four parts: a water trough for containing the films; a sensor for measuring the surface tension difference between a clean-water reference surface and the surface containing the film; a stepper motor mechanism for changing the surface area accessible to the film; and, finally, the computer that runs the instrument, and records and processes data. The design of the sensor, a silicon fiber strain gage, and the interfacing of the instrument to the personal computer are the important innovations in this instrument. Use of the strain gage gives the instrument a usable sensing range of 0.03-30.0 mN/m.

During the past year, two phenomena in monomolecular films have been explored. The first was a study of the phase transition between two "liquid" phases in the film, the "liquid-expanded" and "liquid-compressed" states; the transition was shown to be first order. The second project was the detection of "liquid-vapor" transitions in the films, transitions that occur at very low "pressures" and very dilute surface concentrations.

The film balance will be used over the next year for a detailed study of the phase transition between the "liquid-like" phases and to study "liquid-liquid" immiscibilities in mixed monolayers. These experiments are designed to answer several fundamental questions about the nature of the monomolecular film. Measurements will also be performed on biological films during the next year.

Over the past three and a half years, G. Morrison, R.F. Chang, J.M. Kincaid and I.L. Pegg have been involved in a project to explore the effect of huge surface-to-volume ratios on liquid-vapor phase equilibrium in mixtures; systems such as mists, fogs, clouds, aerosols and sprays fall into this class. Because settling of the droplets impedes the long-time study of such systems, it was anticipated that this study would lead to a microgravity experiment; this work has been supported in part by NASA. In recent experiments, water mists dispersed in an immiscible liquid such as toluene were found to be stable for hours and the droplet motion slowed considerably, allowing study with techniques such as laser Doppler velocimetry. If our NASA proposal is approved, we shall continue our work on these dispersed systems.

Transport Properties of Fluids and Fluid Mixtures

In recent years industry has become increasingly aware that transport properties play a significant role in process design, and that accurate knowledge of these properties can lead to substantial economic benefit.

Thermophysics Division work on transport properties of fluids encompasses the development of new measurement techniques, the utilization of advanced apparatuses to obtain accurate data for transport properties, correlation of available transport property data, theoretical studies of kinetic and transport theory, and the development of wide-range predictive models for transport properties.

In the area of viscosity measurements, R.F. Berg and M.R. Moldover have developed a torsion oscillator to measure the viscosity of fluids at moderate temperatures (-100°C to 100°C) at pressures to 10 MPa at very low frequencies (0.5 Hz) and shear rates (0.05/s). The oscillator is part of a NASA sponsored project for testing the theory of dynamic critical phenomena by means of viscosity measurements in microgravity environments. In addition to the development of a zero-gravity version of the viscometer, measurements have been made on a microemulsion and two mixtures of alkali metals (with A. Voronel of Tel Aviv University). The microemulsion exhibits an unusual viscosity increase which corresponds to an observed electrical conductivity increase. The alkali metals, which have freezing temperatures as low as -80°C, show viscosity increases at least three times what is seen at room temperature.

D.E. Diller (working with L. Van Poolen of Calvin College) has measured the shear viscosities of compressed gaseous and liquid carbon dioxide + ethane mixtures and their pure components with a torsional crystal viscometer at temperatures between 210-320 K and at pressures to 30 MPa. The measurements have been compared to the extended corresponding states model with results similar to those for other mixtures we have examined in the past. The dependences of the fluidity (reciprocal of viscosity) on volume, temperature, and composition have also been examined.

D.E. Diller (with N.V. Frederick) has developed and is now testing a high temperature (600 K), high pressure (70 MPa) torsional crystal viscometer using argon and methane, for which good data are available in the literature. The viscometer makes use of a special high purity quartz for good performance at high temperatures and tungsten springs for suspending the crystal. The measurement system is partially automated. Tests on argon and methane at 300 K are nearly complete. Most of the measurements are within 2% of the best literature values. Similar tests will soon begin at 500 K, the upper temperature limit of most viscosity data for compressed gases.

In the area of thermal conductivity measurements, the transient hot wire method is recognized today as the method of choice for accurate measurements of the thermal conductivity of fluids. H.M. Roder developed a low temperature apparatus which was completed several years ago. It incorporates a long and a compensating short hot wire in different arms of a Wheatstone bridge with control and data logging accomplished by a microcomputer. Roder and D.G. Friend have measured complete surfaces for the thermal conductivity of oxygen, methane, ethane, and methane-ethane mixtures, and partial surfaces for a number of other substances. The physical states measured include the dilute gas, the moderately dense gas, the compressed liquid up to 70 MPa, vapor at temperatures below critical, and a portion of the critical region. The experiment is unique in that one can demonstrate the onset of convection experimentally. Dr. Friend worked with Roder on the mixture measurements and the results clearly show the existence of critical enhancement for the methane-ethane system. Friend is continuing work on the development of a mixture transport model which is theoretically based and can be used for prediction purposes.

At the present time H.M. Roder is developing (with C. Nieto de Castro of Lisbon University) a new apparatus, which will raise the upper temperature limit from 330 K to 775 K. At the same time they have been improving the automation and the resistance measurement in the low temperature system. The immediate goal is to obtain both thermal diffusivity and thermal conductivity from a single experiment. Further into the future, Roder expects to develop a system with coated or insulated wires that allow measurement of polar substances and mixtures.

J.F. Ely is developing theoretically based predictive models for the transport properties of fluid mixtures (emphasis on hydrocarbon and related mixtures) over broad ranges of temperature, pressure, and composition. The work includes the development of the TRAPP computer code, currently distributed by the NBS Office of Standard Reference Data, and which predicts density, thermal conductivity, and viscosity of hydrocarbon mixtures. An expanded version which includes phase equilibria, derived properties, and an improved representation of high density viscosity is in the final stages of development.

J.C. Rainwater and D.G. Friend are working on kinetic theory, with emphasis on the development of a more rigorous and usable theory to predict the viscosity, thermal conductivity, and diffusion coefficients of moderately dense gases. In this area also, a new computer model has been developed to calculate dilute gas collision integrals.

J.V. Sengers (in collaboration with J.C. Nieuwoudt of the University of Maryland and B. Le Neindre and R. Tufeu of CNRS, France) has developed predictive models for the transport properties of isobutane. Dr. Sengers has also developed similar equations for the transport properties of carbon dioxide, with W.A. Wakeham of Imperial College and J.T.R. Watson of NEL, Glasgow. D.G. Friend, B.A. Younglove, J.F. Ely and H.J.M. Hanley are developing correlations and predictive models for the transport properties of hydrocarbons.

Thermophysical Measurements by Dynamic Methods

The goal of this program is to develop and utilize techniques which are capable of highly accurate measurements of thermal, optical, and electrical properties of technically important materials at high temperatures using very high heating rates. Experimental capabilities include millisecond techniques which allow measurements of heat capacity, thermal expansion, electrical resistivity, phase transition points and latent heats, emissivity, etc; microsecond techniques for measuring thermophysical properties at heating rates of 10^7-10^8 K/s; and millisecond techniques for such measurements in a microgravity environment. Plans for the immediate future include the development of dynamic techniques for measurements on nonconducting materials and theoretical studies of dynamic measurement techniques. The program is under the technical direction of A. Cezairliyan.

A. Cezairliyan and A.P. Miiller have completed measurements of the radiance temperature (at 655 nm) of graphite at its triple point using the millisecond-resolution system. The experiments were performed with a pressurized specimen chamber at 20 MPa. The specimen heating rate was about 3×10^5 K/s. The measurements, which are believed to be the most accurate made so far in the world, yield a value of 4330 ± 50 K for the radiance temperature. Work will continue on measurements at other wavelengths with the objective of determining the true triple point temperature of graphite. The triple point of graphite is the highest known solid-liquid transition point and is a potential candidate to become a thermometry fixed point.

A. Cezairliyan, J.L. McClure and M.S. Morse have completed the development and testing of a novel microsecond technique for the measurement of thermal properties of high-melting-point, electrically conducting materials. This marks the culmination of extensive research performed during the past ten years. The new microsecond-resolution system is about 1000 times faster than the millisecond system, permitting heating of specimens at rates of 10^7-10^8 K/s and to temperatures considerably above the melting point of the specimens (up to about 6000 K). The technique utilizes a 20 kV capacitor discharge system and an ultra-fast photoelectric pyrometer specifically developed for this project. This system, unique of its kind in the world, has just recently been used to measure heat of fusion, heat capacity, and electrical resistivity of niobium around its melting point with unprecedented accuracy. Research will continue to extend the measurements to higher temperatures and to other refractory materials, and to investigate nonequilibrium phenomena.

A. Cezairliyan, A.P. Miiller and M.S. Morse are conducting research to develop a system for the measurement of thermophysical properties of liquid electrically conducting substances at high temperatures (above 2000 K) in a microgravity environment. Efforts were concentrated in the study of the geometrical stability of the liquid specimen when heated rapidly by the passage of an electrical current pulse through it in a near-zero-gravity environment. Diagnostic experiments were performed this past year on board a KC-135 aircraft operated by NASA. The experiments on board the aircraft were conducted by P. Giarratano of the Chemical Engineering Science Division in Boulder. Definite excursions in the liquid phase could be seen from the results of the high-speed films and the pyrometric recordings. In order to improve the geometrical stability of the specimen, a triaxial configuration for the specimen and the current leads was studied and an experimental chamber designed. This arrangement would enable balancing of the surface tension and the electromagnetic forces on the specimen. Preparations are underway to perform experiments in KC-135 aircraft utilizing the new chamber.

In somewhat related work, R.A. MacDonald and R.D. Mountain (working with J.E. Callanan, S.A. Sullivan, and K.M. McDermott of the Chemical Engineering Science Division) have conducted theoretical studies using the experimental results of Callanan et al., for the heat capacity of premium coal samples. The work is aimed at providing a predictive model for thermal properties of coal and similar heterogeneous materials. An existing kinetic model for the loss of volatile matter has been compared with the experimental data, for both premium and oxidized samples of coal, and the results are quite dramatic. Related work by Drs. Mountain and MacDonald, which models the stability of type II gas hydrates, is also collaborative with the Chemical Engineering Science Division.

5. HONORS AND AWARDS

James F. Ely - Special Award for Excellence in Technology Transfer, from the Federal Laboratory Consortium for work on supercritical fluid properties, May 1986.

Department of Commerce, Silver Medal Award for outstanding creativity in developing theoretically based predictive models for the thermophysical properties of fluids, November 1986.

Thomas J. Bruno - Department of Commerce, Bronze Medal Award for oustanding leadership in characterizing and measuring the thermophysical properties of reacting fluids, December 1986.

Raymond D. Mountain - Appointed an NBS Fellow, July 1986.

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7. TALKS

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Kayser, R.F., Wetting Layers: Theory and Experiment, University of Maryland Statistical Physics Seminar, University of Maryland, College Park, MD, Apr. 22, 1986.

Kayser, R.F., Wetting of a Binary Liquid Mixture on Glass, Washington Area Statistical Mechanics Meeting, National Bureau of Standards, Gaithersburg, MD, May 6, 1986.

Kayser, R.F., Finite Size Effects on Surface Tension, NBS Staff Research Seminar, National Bureau of Standards, Gaithersburg, MD, May 16, 1986.

Kayser, R.F., Wetting Layers on Ionizable Substrates, Gordon Conference on Chemistry at Interfaces, Meriden, NH, July 24, 1986.

Kayser, R.F., Wetting Layers on Ionizable Substrates, Department of Chemical Engineering, Rensselaer Polytechnical Institute, Troy, NY, Aug. 5, 1986.

Levelt Sengers, J.M.H., Near-Critical Aqueous Electrolyte Solutions, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, Feb. 3, 1986.

Levelt Sengers, J.M.H., Dilute Mixtures and Solutions near Critical Points, 4th International Conference on Fluid Properties and Phase Equilibria for Chemical Process Design, LO-Skolen, Denmark, May 14, 1986.

Levelt Sengers, J.M.H., Aqueous Solutions near the Critical Point of Water, Gordon Conference on Water and Aqueous Solutions, Colby-Sawyer College, NH, Aug. 5, 1986.

Levelt Sengers, J.M.H., Dilute Near-Critical Mixtures and Aqueous Electrolyte Solutions, Van der Waals Laboratory, University of Amsterdam, Netherlands, Sep. 16, 1986.

Levelt Sengers, J.M.H., Dilute Near-Critical Mixtures and Aqueous Electrolyte Solutions, Institute for Physical Chemistry, Ruhr Universitaet, Bochum, W. Germany, Sep. 26, 1986.

McCarty, R.D., The Equation of State for Natural Gas - A Review of Fifteen Years of Progress, Chemical Engineering Science Division Colloquium, NBS/CCE, Boulder, CO, May 16, 1986.

McCarty, R.D., Extended Corresponding States as Applied to Mixtures, 4th International Workshop on Equations of State, University of Idaho, Moscow, ID, Aug. 7, 1986.

Miiller, A.P., A Dynamic Method for Thermophysical Measurements in a Microgravity Environment, The Metallurgical Society 1986 Annual Meeting, New Orleans, LA, Mar. 3, 1986.

Moldover, M.R., Phase Equilibria in the Critical Region, Instituto de Desarrollo Technologico para la Industria Qumica (INTEC), Santa Fe, Argentina, Nov. 8, 1985.

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Moldover, M.R., Wetting, Multilayer Adsorption, and Interface Phase Transitions, Department of Chemistry, University College, London, England, Dec. 11, 1985.

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Moldover, M.R., What Controls the Thickness of Wetting Layers? Faraday Symposium No. 20, Physical Chemistry Laboratory, University of Oxford, London, England, Dec. 18, 1985.

Moldover, M.R., Optical Studies of Interfaces, Department of Physics, Temple University, Philadelphia, PA, Apr. 7, 1986.

Moldover, M.R., Wetting Layers and Interface Phase Transitions, Haverford College, Haverford, PA, Sep. 24, 1986.

Moldover, M.R., Accurate Measurement of the Universal Gas Constant, R, Using an Acoustic Resonator, Haverford College, Haverford, PA, Sep. 25, 1986.

Morrison, G., Impurity Extractions by Droplets, PACE/NASA Symposium, National Academy of Sciences, Washington, DC, Mar. 12, 1986.

Mountain, R.D., Computer Simulation Study of Fluid Mixture Phase Separation in Films, American Institute of Chemical Engineers, Chicago, IL, Nov. 11, 1985.

Nielson, G.C., A Decorated Lattice Gas Model for Supercritical Solubility, Statistical Physics Colloquium, Catholic University, Washington, DC, Apr. 4, 1986.

Paulaitis, M.E., Multiphase Behavior in Ternary Mixtures at Elevated Pressures, Chemical Engineering Science Division Colloquium, NBS/CCE, Boulder, CO, Apr. 25, 1986.

Rainwater, J.C., Vapor-Liquid Equilibrium of Binary Mixtures, Cornell University, Ithaca, NY, Sep. 26, 1986.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

P.C. Albright

NBS Child Care Center (Board of Directors)

A. Cezairliyan

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

Thermophysical Properties Committee K-7 of the American Society of Mechanical Engineers (Member)

International Thermophysics Congress (Chairman)

International Commission on Standardization of Thermophysical Measurement Techniques (Member)

Thermophysical Properties Subcommittee of ASTM (Member)

E.J. Clark

ASTM E44 Committee on Solar Energy (Member)

ASTM G3 Committee on Durability of Nonmetallic Materials (Member)

D.E. Diller

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

J.F. Ely

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

Gas Processors Association Data Book Revision Committee (Member)

NBS Research Advisory Committee (Member)

Boulder Computer Users Group (Member)

D.G. Friend

Boulder Editorial Review Board (Member)

L. Haar

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

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

NBS Library Committee (Member)

NBS Editorial Review Board (Member)

H.J.M. Hanley

ASME Thermophysical Properties Committee (Member)

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

J.B. Hubbard

NBS Colloquia Committee (Member)

N.A.T.O. Advanced Study Institute Publication Committee (Member)

J.M. Kincaid

NBS Storeroom Committee for ADP (Chairman)

J.M.H. Levelt Sengers

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

ASME Research Committee on the Properties of Steam (Member)

G. Morrison

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

R.D. Mountain

NBS Library Subject Specialist Committee (Member)

NBS User Committee for Scientific Computing (Chairman)

N.A. Olien

ASTM D-3 Committee on Gaseous Fuels (Member)

ASTM E-49 Committee on Computerization of Material Property Data (Member)

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

IUPAC Committee on Transport Properties (Corresponding Member)

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

Meeting Program Chairman, AIChE National Meeting, Denver, CO, Aug. 21-24, 1988

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)

J.V. Sengers

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

ASME Research Committee on the Properties of Steam (Member)

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

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

International Review Panel to evaluate the F.O.M. - scientific program on molecular physics in The Netherlands (Member)

B.A. Younglove

Thermophysics Division Hazards Review Committee (Member)

EDITORSHIPS

T.J. Bruno

Handbook, Basic Tables for Chemical Analysis, CRC Press (Co-editor with P.D.N. Svoronos)

A. Cezairliyan

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

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

International Journal of Thermophysics (Editor-in-Chief)

Journal of High Temperature Science (Editorial Board)

Journal of High Temperatures-High Pressures (Editorial Board)

H.J.M. Hanley

NBS Journal of Research (Boulder Editor)

International Journal of Thermophysics (Editorial Board)

W.M. Haynes

Cryogenics (U.S. Advisory Editor)

A.P. Miiller

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

N.A. Olien

Journal of Physical and Chemical Reference Data (Editorial Board)

J.V. Sengers

Physica A (Editorial Board)

International Journal of Thermophysics (Editorial Board)

Royal Dutch Academy of Science (Correspondent)

9. PROFESSIONAL INTERACTIONS

FACULTY APPOINTMENTS

T.J. Bruno

Adjunct Associate Professor, Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines

J.F. Ely

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

H.J.M. Hanley

Professor Adjoint, Department of Chemical Engineering, University of Colorado

M.R. Moldover

Adjunct Professor, Institute for Physical Sciences and Technology, University of Maryland

J.C. Rainwater

Associate Professor Adjoint, Department of Physics, University of Colorado

INDUSTRY

J.F. Ely

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

Technical Manager of industrial consortium and collaboration with member companies involved: Air Products and Chemicals, Inc., ARCO Transportation Company, Bessemer Reciprocating, Enron, Gas Processors Association, Mobil Research and Development Corporation, Phillips Petroleum Company, Shell Development Company, SOHIO, and Ingersoll-Rand Company, on measurement and prediction of fluid properties.

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

H.J.M. Hanley

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

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

J.W. Magee

Collaboration with steering committee of industrial consortium whose member companies are: ARCO Transportation Company, Bessemer Reciprocating, Gas Processors Association, Mobil Research and Development Corporation, Enron, Phillips Petroleum Company, and Ingersoll-Rand Company, on measurements of CO_2-rich mixture properties.

M.R. Moldover

Collaboration with J. Huang, Exxon Research and Engineering Company, Florham Park, NJ, on measurements of transport properties of microemulsions.

J.C. Rainwater

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

ACADEME, NATIONAL LABORATORIES AND GOVERNMENT

T.J. Bruno

Cooperative research with D.E. Martire, Department of Chemistry, Georgetown University, Washington, DC, on supercritical fluid chromatography.

Coauthor of books on analytical chemistry with P.D.N. Svoronos, City University of New York, NY.

A. Cezairliyan

Cooperative research with the Italian Metrology Institute, Torino, Italy, on melting point measurements.

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.

D.E. Diller

Cooperative research with C.A. Nieto de Castro and F. dos Santos, University of Lisbon, Lisbon, Portugal, on development of a high pressure (300 MPa) viscometer for liquids.

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

J.F. Ely

Cooperative research with T. Leland and D. Erickson, Department of Chemical Engineering, Rice University, Houston, TX, on hard sphere expansion theory for polar and nonpolar fluid mixtures and rescaling of classical equations of state.

Cooperative research with A. Mansoori, Department of Chemical Engineering, University of Illinois, Chicago, IL, on local composition models and Kirkwood-Buff theory for fluid thermodynamic behavior.

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

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

H.J.M. Hanley

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

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

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

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

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

W.M. Haynes

Cooperative research with J.C. Holste, Department of Chemical Engineering, 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.

Cooperative research with D.W. Kupke, Department of Biochemistry, University of Virginia, Charlottesville, VA, on magnetic suspension densimetry and viscometry.

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

J.B. Hubbard

Collaboration with P.J. Stiles, Macquarie University, Australia, and H. Brenner, M.I.T., Boston, MA, on hydrodynamics of magnetic and dielectric colloidal suspensions.

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

Collaboration with J. Rasaiah and S.H. Lee, University of Maine, Orono, ME, and R. Rubin, NBS/CCP, Gaithersburg, MD, on diffusion-controlled reaction kinetics - theory and computer simulations.

Collaboration with A. McCammon, University of Houston, Houston, TX, on the internal dynamics of proteins.

Collaboration with H. Friedman, SUNY, Stony Brook, NY, on the statistical physics of electrolyte solutions.

J.M. Kincaid

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

Cooperative research with E.G.D. Cohen and M. Lopez de Haro of Rockefeller University, New York, NY, on kinetic theory.

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

J.M.H. Levelt Sengers

Received NATO grant jointly with J. de Swaan Arons, University of Delft, Netherlands, to study and model near- and supercritical polymer solutions. Collaborators L. Clark, P.H.E. Meijer, I. Pegg and C. Peters (Delft).

Joint paper with K.S. Pitzer, University of California, Berkeley, CA, on properties of near-critical aqueous salt solutions.

Joint proposals with P. Meijer and I. Pegg, Catholic University, Washington, DC, in the area of polymer solutions. Collaborator L. Clark, Consultant M. McHugh, Johns Hopkins University, Washington, DC.

Collaboration with R. Fernandez-Prini, CNEA, Argentina. R. Fernandez-Prini is planning to send a coworker as guest scientist to NBS.

Collaboration with J. Straub, University of Munchen, Munchen, West Germany, to formulate the refractive index of water and steam in terms of the HGK equation. J. Straub will send a student to do this work at NBS.

Collaboration with W. A. Wakeham, Imperial College, London, England, R. T. Jacobsen, University of Idaho, Moscow, Idaho, R. McCarty, NBS/CCE, Boulder, CO, and J.V. Sengers, NBS/CCE, Gaithersburg, MD, to publish an IUPAC book on the properties of ethylene.

R.A. MacDonald

Collaboration with J.M. Kincaid, Dept. of Mech. Eng., SUNY, Stony Brook, NY, on thermodynamics of multicomponent and polydisperse mixtures.

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

J.W. Magee

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

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

R.D. McCarty

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

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

M.R. Moldover

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

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

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

G. Morrison

Collaboration with J.C. Wheeler, University of California, San Diego, CA, on the origin of several "paradoxical" features of phase diagrams near "non-classical" critical points in mixtures.

Collaboration with J.M. Kincaid, Dept. of Mech. Eng., SUNY, Stony Brook, NY, on the thermodynamics of polydisperse systems.

Collaboration with D.A. Didion, M.O. McLinden, and B. Mahajan, NBS/CBT, Gaithersburg, MD, on refrigerant mixture properties and modeling.

R.D. Mountain

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

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

N.A. Olien

Joint Chairmanship of Symposium on Thermodynamics for Bioseparations at November 1987 AIChE National Meeting with Professor Carol Hall, Department of Chemical Engineering, North Carolina State University, Raleigh, NC.

J.C. Rainwater

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

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

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

Collaborative research with W.B. Kay, Department of Chemical Engineering, Ohio State University, Columbus, OH, on vapor-liquid equilibrium of binary mixtures.

Collaborative research with R.T. Jacobsen, Center for Applied Thermodynamic Studies, University of Idaho, Moscow, ID, on the coexistence surface of air.

Collaborative research with J.A. Zollweg, School of Chemical Engineering, Cornell University, Ithaca, NY, on vapor-liquid equilibrium of binary mixtures.

H.M. Roder

Cooperative research with W.A. Wakeham, Department of Chemical Engineering, Imperial College, London, England, on thermal conductivity of fluids.

Cooperative research with C.A. Nieto de Castro and U.V. Mardolcar, Department of Chemistry, University of Lisbon, Portugal, on measurements of thermal conductivity.

Cooperative research with J. Venart and R.C. Prasad, Department of Mechanical Engineering, University of New Brunswick, Canada, on thermal conductivity.

G.C. Straty

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

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

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

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

WORKSHOPS

Working Group A, International Association for Properties of Steam, held at Dusseldorf, FRG, Sept. 21-26, 1986. Chaired by J.M.H. Levelt Sengers, who also coorganized a one-day workshop on aqueous systems during this week.

SEMINARS

F. Larche, Physics Department, University of Montpellier, Montpellier, France: Phase Behavior and Organized Structures in a Ternary Surfactant-Water-Alcohol Solution, Oct. 23, 1985.

S. Finke, Chemical Engineering Department, Ohio State University, Columbus, OH: Recent Phase Behavior Studies at Ohio State University, An Experimental Overview, Oct. 28, 1985.

D. Beyssens, Service de Physique du Solide, Saclay, France: Adsorption Phenomena in a Binary Fluid using Silica Spheres, Nov. 7, 1985.

B.M. Law, Institute for Physical Science and Technology, University of Maryland, College Park, MD: Are Current Theories of Wetting Correct?, Nov. 27, 1985.

B. Volintine, Chemical Engineering Department, Rensselaer Polytechnic Institute, Troy, NY: Interfacial Heat Transfer, Dec. 5, 1985.

D. Roux, Exxon Research and Engineering Company, Annandale, NJ: Critical Behavior and Spinodal Decomposition in Microemulsions, Dec. 9, 1985.

D. Beysens, Service de Physique du Solide, Saclay, France: Recent Progress in Probing Wetting Layers by Means of Silica Colloids, Jan. 27, 1986.

P.B. Balbuena, Universidad Nacional del Litoral, Santa Fe, Argentina: Calculations of VLE near Critical Points using Scaling EOS Combined with Van der Waals Type EOS, Feb. 12, 1986.

S.W. Churchill, University of Pennsylvania, Philadelphia, PA: Computation of 3-Dimensional Natural Convection in Enclosures, Feb. 21, 1986.

B.U. Felderhof, Institut fur Theoretische Physik, Technische Hochschule Aachen, W. Germany: Hall Effect in Water, Mar. 10, 1986.

J.P.M. Trusler, University College, London, England: Redetermination of the Gas Constant, Mar. 26, 1986.

V. Steinberg, Weizmann Institute of Science, Rehovot, Israel: Experiments on Convection in Binary Fluid Mixtures Heated from Below, Mar. 31, 1986.

M.E. Paulaitis, Department of Chemical Engineering, University of Delaware, Newark, DE: Multiphase Behavior in Ternary Mixtures at Elevated Pressures, Apr. 25, 1986.

G. Grimvall, Department of Theoretical Physics, The Royal Institute of Technology, Stockholm, Sweden: Thermophysical Properties - Can Theoretical Calculations be an Alternative to Direct Measurements?, May 2, 1986.

N.N. Li, Separation Science and Technology, Signal Research Center, Des Plaines, IL: Future Separation Technologies, May 30, 1986.

G. Chou, Chemical Engineering Department, University of California at Berkely, Berkeley, CA: Developments in Continuous Thermodynamics, June 9, 1986.

R. Guy, University of California, San Francisco, CA: Interfacial Transport: Rotating Diffusion Cell and Capillary Tube Techniques, June 13, 1986.

J.A. Schouten, Van der Waals Laboratory, University of Amsterdam, Amsterdam, Netherlands: Visual Observation of Phase Separations in Fluid Mixtures, June 20, 1986.

H. Cabezas, Jr., Chemical Engineering Department, University of Arizona, Tucson, AZ: Fluctuation Solution Theory Models of Electrolyte and Biopolymer Solutions, June 23, 1986.

E. Gulari, Chemical Engineering Department, Wayne State University, Detroit, MI: Supercritical Extraction and Light Scattering in Polymer Solutions, June 27, 1986.

E.S.R. Gopal, Instrumentation and Service Unit, Indian Institute of Science, India: Critical Wetting Phenomena, July 28, 1986.

C. Franck, Physics Department, Cornell University, Ithaca, NY: Wetting Experiments of Binary Liquid Mixtures on Solid Substrates, Aug. 22, 1986.

A. Voronel, Physics Department, Tel Aviv University, Ramat Aviv Israel: Freezing of Alkali Metal Alloys, Sep. 2, 1986.

A. Voronel, Physics Department, Tel Aviv University, Ramat, Aviv, Israel: Structural Phase Transitions in Alkali Metal Alloys, Sep. 4, 1986.

B. Smit, Chemical Technology, Technical University Delft, Holland: Thermodynamic Modeling of the Water-Oil-Surfactant System using the 2-suffix Margules Equation, Sep. 9, 1986.

G. Ernst, University of Karlsruhe, W. Germany: Experimental Determination of the Specific Heat Capacity of Water at Temperatures between 25°C and 400°C and Pressures between 200 bar and 500 bars, Sep. 10, 1986.

S. Abramowitz, NBS, Center for Chemical Physics, Gaithersburg, MD: Biotechnology Research in the NBS-Center for Chemical Physics, Sep. 15, 1986.

P.E. Phillips, Professional Nutrition Services, Boulder, CO: Nutrition and Immunity, Sep. 26, 1986.

TECHNICAL ACTIVITIES OF THE CHEMICAL PROCESS METROLOGY DIVISION

J.J. Ulbrecht, Chief

1. INTRODUCTION

A common denominator of all research projects carried out in the Chemical Process Metrology Division in this past fiscal year was a sustained effort to bring the research output closer to the needs of the chemical and related industries.

Emphasis has been placed on employing the principles of engineering science to develop new techniques for process sensing, diagnostics and metrology and to obtain new data for process control and process design.

The current mixture of research projects consists of some new projects and some continuing ones. The measurement of flow birefringence by guided microwaves and the numerical simulation of chemically reacting flows are some of the new ventures started this past year. Both projects hold promise for a wide application of their respective results, the former particularly in the polymer and coating technologies, the latter in high temperature reactions.

Significant progress is being reported in a number of continuing projects. Optical diagnostic techniques for bioreactors have been used to identify a sequence of amino acids in dipeptides and polypeptides. The construction of the plug flow reactor has been completed and the fluidized bed reactor is being tested for the incineration of chlorinated hydrocarbons. A new experimental technique has been developed to study formation of silica particles in flames, and we expect to extend this work to include gas phase diagnostics for microcircuit fabrication.

New and exciting results were obtained in applying the laser tomographic technique to transient processes. The three-dimensional reconstruction of the reaction field revealed some features of coherent turbulent structures not seen before. Also the particle and droplet diagnostic technique has come of age and new data were obtained.

Last year, after some delays, the new surface analytical facility came on stream. During the past year, this facility was extensively used to study some of the surface characteristics of tin oxide and iridium oxide. Among the features studied is the unusual semicrystalline form of iridium oxide that makes this material suitable for ionic sensing. In the future, we expect this sensing material to have broad application in all chemical reactions involving exchange of protons.

Two of our existing projects reached the stage of prototype testing: the RF sensor for the measurement of solids fraction in flowing slurries was tested under plant conditions and the spectroscopic temperature probe is being readied for plant tests at the time of the writing of this report. Results obtained so far are encouraging and a successful completion of these two projects can be expected soon.

Among the projects successfully completed was the upgrade of all calibration facilities. This project required major concentration of material and human resources and its completion represents a significant achievement.

The Division has been striving to develop and maintain all possible forms of technology transfer. Industrial consortia have been one of the most successful forms of this transfer and the "Installation Effects" consortium has attracted a substantial membership. The results are reported in the main body of this report.

The Division continued providing calibration services in mass and volumetric flow, air speed, humidity, volume and liquid density to industrial and public clients across the country. The recent upgrading of these facilities will make it possible to serve the U.S. industry even better.

2. GOAL

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

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

A key element in the pursuit of this goal is the study of the surface, transport, and kinetic phenomena in the environment of sensing and diagnostic tools.

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

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

3. GROUP FUNCTIONS

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

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

Research is primarily focused on flow phenomena in confined flows as well as in free surface flows in geometries pertinent to the technologies used in the chemical and related industries.

The Fluid Flow Group maintains responsibility for the fluid flow rate and airspeed calibration services and for the maintenance and upgrading of the relevant national standards. The Group is responsible for the transfer of fluid flow measurement technology to industry and to public institutions.

* Multiphase Reacting Flows Group - A.K. Gaigalas, Group Leader

The mission of the Multiphase Reacting Flows Group is 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 for on-line process diagnostics, and (3) develop mathematical models for improved understanding and control of physical, chemical, and biochemical processes.

Particular emphasis is placed on the development of advanced diagnostic techniques utilizing electromagnetic and acoustic fields and electrochemical phenomena.

The Multiphase Reacting Flows Group bears the responsibility for NBS calibration services in liquid density and volume.

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

The High Temperature Reacting Flows Group conducts fundamental research on chemically reacting flows, especially those with gas-solid reactions involving solid particles either formed or entrained. The research includes advanced optical, non-intrusive measurement techniques for high temperature reactors such as combustors and fluidized bed reactors.

Particular emphasis is on the use of laser scattering and extinction techniques for particle characterization, on laser tomography for temperature and composition measurement, laser induced fluorescence (LIF), and emission spectroscopy for temperature measurement.

The scattering/extinction techniques are being adopted for the study of gas-solid chemical reactions relevant to chemical vapor deposition, and to ceramics and powder metallurgy.

A significant segment of the research activities in this group is the extension of the LIF techniques to optical diagnostics of species (nutrients, substrates, metabolic intermediates, and products) in biochemical reactors.

A new laboratory facility has been completed to study transport and reaction rates in multiphase flow systems relevant to pyrolysis and oxidation.

* Process Sensing Group - J.R. Whetstone, Group Leader

The Process Sensing Group performs research directed toward the development of process sensors with particular emphasis on solid state sensors for chemical species, humidity and temperature. Reactive sputtering is used to form films and a comprehensive surface analytical facility is used to characterize the surfaces of these films where the chemical reaction takes place.

For gas sensing, the focus of the research is on tin oxide films while iridium oxide forms the backbone of the work on ionic sensors. Further, thin film thermocouples deposited on metal, ceramic and polymer substrates are the subject of study.

A study to develop optimization and standardization of methodology for collection of samples of water, air, and soil is an integral part of the research effort in this group.

The Process Sensing Group is responsible for providing the NBS calibration services for humidity and for the maintenance of the humidity national standard.

4. SELECTED PROJECT SUMMARIES

CALIBRATION SERVICES

Calibration and Test Services Performed by the Chemical Process Metrology Division

G.E. Mattingly, A.K. Gaigalas, K.G. Kreider

In the past year, the CCE calibration services have satisfied industry and government requests for a number of metrological tasks in the areas of fluid flowrate, liquid density and volume, air speed, and humidity measurements. Additionally, the techniques and facilities for performing these services have been upgraded so that the levels of measurement uncertainty are quantified and reported for publication in the appropriate literature. In the specific calibration services offered to U.S. industry, activities are summarized as follows:

Service	Number of Items Calibrated
Flowrate	29 (29 for industry)
Volumetric Containers	55 (53 for industry)
Aerodynamic Devices	83 (58 for industry)
Reference Standard Hydrometers	2 (2 for industry)
Humidity	47 (31 for industry)

These calibrations generally establish a traceability link between the respective calibration requester and NBS. In this way, these calibrations form a basis for the assurance of all the measurements produced in the requester's laboratories.

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

In the last year, NBS has responded to a DoD request for a round-robin flow measurement program to be designed and carried out to check flowmeter calibration facility performance in Army, Navy, and Air Force labs. This program, requested for hydrocarbon liquids, has been designed for several sets of tandem turbine meters. Specific test procedures have been developed and approved by the DoD labs so that Youden analyses can be used to analyze the data and to quantify lab performances. The program, once established and demonstrated, will be used on a continuing basis to maintain desired control of these measurement processes. In this manner, realistic flow measurement traceability will be established and maintained for the participating labs.

FLUID FLOW GROUP

Flowmeter Installation-Effects Research

G.E. Mattingly, T.T. Yeh

An NBS-DoE funded flowmeter research program on installation-effects progressed to the point of attracting participation of industry through a consortium that has been formed to assist in supporting this program. Benefits to consortium participants are guiding current and future phases of the work and receiving results on a timely basis. The consortium has grown to thirteen meter manufacturers and users - U.S. and foreign. Research results are intended to upgrade or to initiate useful installation specifications for flowmetering standards by implementing a new strategy to achieve this goal.

The strategy adopted for this program contrasts markedly with that used in the past. Conventionally, it has been the practice to conduct very considerable numbers of specific meter calibrations to determine the minimal distances (between meter and specific upstream piping configuration) for which uncertainty levels on meter factors are to be increased by specified amounts. Through this conventional approach, little was learned or understood of the salient features of the pipeflow profiles involved. The currently adopted strategy focuses on these profiles, specifically, measures them using Laser Doppler Velocimetry (LDV), and characterizes them and their changes with distance from the piping configuration.

With these results, and the associated understanding, a number of limited, informed calibration tests can be carried out by meter manufacturers and others so that specific results, i.e., discharge coefficients, meter factors, etc., are thereby related to pertinent pipeflow characteristics. In this way, meters can be installed in any locations where their performance is satisfactorily stable and meter factors or discharge coefficients are satisfactorily predicted for the installation. It is expected that this strategy will produce installation specifications for metering standards which will enable satisfactory flow measurements to be made in installations previously considered non-ideal and for which no current standards are applicable.

In the past year, extensive LDV profiling has been done in two-inch (50 mm) diameter, cylindrical pipeline water flows. Results for diametral Reynolds numbers of 10^4 and 10^5, and a relative roughness of 0.0005, show that the selected elbows-out-of-plane configuration generates severe and complex swirl. This swirl initially resides off the pipe centerline and only in the regions near the pipe walls. (These results indicate that a specialized flow conditioning element may effectively eliminate or significantly reduce this swirl before it diffuses over the entire cross-sectional area of the pipe.) In the piping downstream from this configuration, the severe swirl, initially near the pipewall, is found to diffuse over the pipe cross-section and "spin-up" the center core region of the pipeflow. Following this, the swirl distribution diffuses with downstream distance, but this process requires considerable lengths of pipe. For our selected smooth pipe conditions, this swirl produces "swirl angle" (velocity vector inclination) levels of up to 3° at 95 diameters from the perturbing configuration.

For three different types of flowmeters (orifice, turbine, and vortex shedder) the methodology of our research was demonstrated. The success level varied for the different types of flowmeter. Greater success was found with the turbine meter. In spite of enormous shifts produced in its meter factor by the severe swirl, limited calibration results (<u>with the understanding produced via our LDV measurements</u>) enabled accurate predictions to be made for its meter factor in "non-ideal" installations. Less success was attained with the other types of meters.

It is concluded that this strategy for producing improved flowmeter installation specifications can be very effective. Successive phases of the research, if supported at current levels, can continue to produce analogous results for commonly used piping configurations so well known to disrupt "ideal" meter performance. It is also concluded that results of this program can be very useful in designing and installing efficient flow conditioners for reducing or eliminating such anomalous pipeflows.

MULTIPHASE REACTING FLOWS GROUP

Measurement of Birefringence at Microwave Frequencies

A.K. Gaigalas, J.J. Ulbrecht

The purpose of this project is to design and fabricate a sensor with sufficient sensitivity to detect small dielectric differences associated with two directions in an anisotropic material. The motivation for this research is in the need to develop an on-line measurement of viscoelasticity in polymers, in polymer composites, and in other materials with preferred orientation.

A hairpin line was selected because theoretical considerations showed that its propagation characteristics are very sensitive to the properties of the material on top of the line. By placing two hairpin lines oriented at right angles to each other, in a flow of polymeric material, it should be possible to detect flow induced anisotropy in the dielectric constant and hence the normal stress. The main effort was in modeling of the hairpin line response. Since the hairpin line is a bandpass device and since the width of the bandpass is a sensitive function of the coupling between adjacent strips in the hairpin line, it is crucial that the theoretical description of the coupling is accurate. At this point we have tried the thin line approximation to describe the hairpin line. The model predicts the frequency of the center of the bandpass, but the prediction of the bandpass width is not very accurate. The work is continuing to build a better model and concurrently to fabricate hairpin lines with progressively larger conductor strip densities.

Interaction of Microwaves with Cells

S. Woo, A.K. Gaigalas

A study is being carried out on the interaction of cells with reactive species produced by radio frequency discharges. Atomic species of oxygen, hydrogen, and nitrogen are known to react vigorously in the presence of organic compounds hence it is expected that glow discharge will adversely affect cellular structure. Preliminary work has shown that exposure to glow discharge caused cell death. Work continues to separate ultraviolet effects from atomic gas effects. The knowledge gained from the separation experiment, along with detailed knowledge of cellular structure, will be used to develop mechanisms to investigate cell death. Possible applications of these studies are continuous sterilization of gases and advanced separation techniques for recovery of inorganic substances digested and concentrated by unicellular organisms.

Measurement of Shear Rate Near a Stirring Blade

B. Robertson

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

The shear rate S measured on the front surface of a Rushton turbine blade is correlated by

$$S / N = 3.3 \, (N D^2 / \nu)^{1/2},$$

where N is the turbine rotation rate, D is the turbine diameter, and ν is the kinematic viscosity. This correlation differs significantly from the estimate of the average shear rate in a stirred tank,

$$S / N = 11,$$

by Metzner and Otto (1957). Our measurements from Reynolds number 100 to 30 000 show that the local shear rate on the blade is proportional to the 3/2 power of N, rather than being linear in N as is the case with the average shear rate. Our dimensional analysis shows that S is proportional to D and depends on the kinematic viscosity as shown above. The measured local shear rate is as much as 50 times larger than the average.

Drop Extension and Breakup in Mixer Blade Flow Fields

R.C. Calabrese, B.J. Sadoff

A liquid-liquid drop dispersion flow loop facility has been used, in collaboration with the University of Maryland, to study the deformation and breakup of drops in the vicinity of sharp-edged bodies which simulate real mixing elements. The facility uses laser velocimetry, high speed photography, and the hydrogen-bubble technique to characterize flow fields and drop behavior. Initial laser velocimeter results, for the unobstructed test section, suggest that the settling chamber and converging section are removing large scale turbulence and providing desirable velocity profiles. The early data also indicated that the hydrogen bubble technique must be used to visualize the flow around the blade before taking further laser velocimetry measurements. The flow visualization technique will permit crude studies of velocity gradient and shear fields. The preliminary studies will dictate which areas around the blade must be studied further and, after complete characterization of the flow, drops will be added to allow study of the deformation and breakup process. A mechanistic model for drop stability is being developed concurrently.

On-Line Solid-Phase Fraction Measurement

A.K. Gaigalas, W.G. Cleveland, Jr.

The objective of this project is the development of an accurate, non-intrusive measurement technique for on-line global sensing of solid-phase fractions (consistency) in paper pulp flows. The technique utilizes interference between electromagnetic waves propagating in a waveguide. The waveguide is a part of the piping system carrying the slurry. Recent efforts were directed toward scaling up the technique to a six-inch diameter pipe size. A prototype was constructed and has been successfully tested in the pulp loop at the Institute for Paper Chemistry in Appleton, WI. A large effort has been made to design and fabricate a solid-phase-fraction meter for operation in a paper mill environment. Improvement in the efficiency of the antenna and the reliability of the detection circuitry has been achieved.

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

K. Yuk, J.J. Ulbrecht

The mechanism of gas dispersion in liquid in a stirred tank is simulated by a rotating flow past a stationary blade. The gas cavity behind the stationary blade is formed by feeding air directly into the downstream side of the blade, and is found to be similar to those observed behind rotating stirrers. The local size distribution of the gas bubbles redispersed from the top of the cavity were determined photographically. The effect of Newtonian and non-Newtonian liquid properties and flow parameters on the bubble size is also investigated. The force acting on the blade is measured by a strain gauge mounted on the blade arm. A correlation is being developed between the power dissipated in the wake and the maximum bubble size.

HIGH TEMPERATURE REACTING FLOWS GROUP

Particle Formation in High Temperature Processes

R.J. Santoro, J.J. Horvath, J.L. Katz*, D. Chin*, H.G. Semerjian

Non-intrusive laser diagnostics are being applied to investigate particle formation processes in hydrocarbon flames. Detailed measurements of the soot particle field using laser light scattering techniques have been obtained for a series of laminar diffusion flames. Complementary temperature and velocity measurements have been made in order to examine the effects of variations in the temperature and particle residence time on the soot growth process. Independent variation of the temperature in the flames has been investigated through the addition of inert diluents to the fuel and air flows. The experiments have demonstrated the strong temperature sensitivity of the soot formation process. Studies involving a series of fuel species (ethene, ethane, and methane), as well as a range of fuel flow rates, have elucidated the mechanisms responsible for soot particle escape from these flames. The importance of radiative transfer in establishing conditions conducive to soot particle production has been identified. The results of detailed soot growth calculations based on these studies are being used to form the basis of a soot formation model. More recently, experiments have been extended to a wider range of fuels, including acetylene, propene, and butene, to examine the effect of fuel structure on soot formation. In these experiments, the total amount of fuel carbon has been kept constant by using a base flame of ethane to which various fuels are added. The effect of species concentration on soot formation was studied by addition of nitrogen or argon to obtain the same flame temperature. Temperatures were verified by using a new rapid thermocouple insertion technique. A laboratory-constructed vaporization system was also used to extend the studies of particulate formation processes to heavier fuels, such as toluene. These studies are intended to examine soot formation under conditions more directly related to practical systems.

Efforts are also underway to investigate formation of noncarbonaceous particles. Using a counterflow diffusion flame, formation and growth of silicon dioxide particles are being examined. In these experiments, silane is introduced into a hydrogen-oxygen flame, which provides a flat, highly uniform environment suitable for optical probing. Laser scattering techniques are used to measure particle size and number density, and pulsed-laser methods are used to determine the concentration of intermediate compounds such as SiO and OH. Electron microscopy also is being used to examine particles sampled from the flame.

*Johns Hopkins University

Particulate and Droplet Diagnostics in Spray Flames

C. Presser, A.K. Gupta*, H.G. Semerjian, R.J. Santoro

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

Current efforts are focused on laser scattering and Doppler velocimetry measurements, which are being used to determine the correlation between droplet size and velocity distributions, respectively, in both low temperature and burning sprays. Measurements of the spatial profiles of mean droplet size and number density have been completed, along with fine-wire thermocouple measurements in a pressure-atomized hollow cone spray under nonswirling and swirling conditions. To provide a comparative evaluation of different diagnostic techniques, data on droplet size and number density have been obtained using three different methods: (a) an ensemble light scattering technique, based on measurement of the polarization ratio of scattered laser light; (b) phase/Doppler interferometry, a single particle counting technique; and (c) a light intensity deconvolution technique, another single particle counting method. Laser velocimetry measurements have resulted in measurement of complete spatial profiles of each velocity component (axial, radial and tangential) for both the droplet and combustion air flow fields. Data taken at the burner exit have already been used in the modeling efforts underway at LANL, resulting in good initial agreement between the experimental and numerical results. The quantitative data have also been complimented with different flow visualization techniques which include high speed cinematography, still photography, and video movies. It has been found that the presence of swirl has a significant influence on the spray structure. Comparison of different droplet sizing techniques has demonstrated a disparity in measured droplet size which is attributed to their different dynamic ranges. Efforts are now underway to study fuel property effects. A twin-fluid research atomizer has been fabricated so that spray dynamics can be studied in a well characterized nozzle. An investigation has also been initiated to determine the feasibility of using the polarization ratio technique as a single particle counter.

A collaborative program, to investigate the effect of coalescence and preferential vaporization on droplet size distribution, is being developed with Technion, the Israel Institute of Technology in Haifa. Another collaborative research program has been initiated, with the NBS Institute for Materials Science and Engineering, to apply laser diagnostic techniques to investigate metal powder atomization and rapid solidification processes.

*University of Maryland

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

H.G. Semerjian, S.R. Ray

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

Current work has focused on rapid measurements in non-symmetric fields at repetition rates up to 10 kHz, using a six angle tomography approach. The new system has been used to measure the particle concentration field in rapidly fluctuating flames. Data have been obtained on the dynamics and three-dimensional structure of large eddies formed in an ethene-air turbulent diffusion flame. The frequency of eddy formation is controlled by introducing fluctuations into the fuel stream, using a loudspeaker. The formation, shedding, and break-up of eddies, marked by the soot particles formed in the flame, have been observed with a time resolution of 1 ms. As a parallel effort, a number of alternative reconstruction techniques have been investigated using computer simulations, to identify the approach ideally suited to this experiment. The maximum entropy method is found to be the most suitable, especially for reconstructing the field from a small number of projections (e.g. six angles).

Numerical Modeling of High Temperature Reacting Flows

R.W. Davis, E.F. Moore

High temperature reacting flows are, in general, typified by strong coupling between fluid mechanical and chemical kinetic processes. In most practical systems, such reacting flows are characterized by large fluctuations in species concentration and temperature which occur over small spatial intervals. In order to gain an improved understanding of such complex reacting flows, a joint numerical-experimental program is being carried out. Because of its simple flow configuration, the focus of the initial effort is the laminar axisymmetric diffusion flame. A computer code is currently being developed to model this system. A flame-sheet formulation is being used initially, with the addition of simple chemical kinetics being anticipated at a later date. This model will provide a complete description of the flow, species, and thermophysical properties fields, and permit quick assessment of the effects of parameter variation. Experimental verification efforts are being carried out both within NBS and among outside collaborators. Rigorous comparisons between numerical and experimental results will be made at each level of code development to ensure that the model provides the capability to predict the features of realistic flow fields.

Optical Sensing in Bioreactors

J.J. Horvath, K.P. Brown*, H.G. Semerjian, A.E. Humphrey*

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

Optical techniques, especially with the use of tunable lasers, provide the best potential for making nonintrusive, rapid, and selective measurements. Use of fiber optics can also enable the development of probes which are sterilizable, can provide measurements with good spatial resolution, and can be multiplexed to provide multipoint monitoring capability. Laser induced fluorescence, Raman scattering, and infrared absorption techniques will be utilized for measurement of key process variables such as cell mass activity, cell concentration, and concentration of substrates and products. Experiments have been carried out on fluorescence characteristics of the aromatic amino acids, indicating good sensitivity and selectivity. The fluorescence characteristics of a series of dipeptides and polypeptides were studied to determine the effects of amino acide sequence and various chemical functional groups on the observed fluorescence spectra. The spectra of commercially produced biomolecules such as antibiotics and artificial sweeteners were also observed. The fluorescence spectra of the components of a typical fermentation, i.e. yeast, nutrient, and the product enzyme, have been examined and characterized as a function of excitation wavelength. Present work involves the initial set up and operation of a laboratory scale fermenter, measurements on samples from a fermentation run, and the development of an on-line measurement system. Fluorescence techniques are also expected to provide a powerful tool for cell activity and intracellular kinetics measurements. In the future, Raman and resonance Raman scattering will be utilized to provide improved species selectivity.

*Lehigh University

Emission Spectroscopy for Control of Combustion Systems

S.R. Charagundla, H.G. Semerjian

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

One application of the on-going emission spectroscopy work is in the black liquor recovery boiler. Investigations thus far have characterized the emission spectra (from actual black liquor recovery boilers) in the wavelength range of 300 nm to 800 nm, using a spectrometer equipped with an Optical Multichannel Analyzer (OMA). These data indicate that only the line emissions from sodium at 589 nm, mostly in self-absorption, and from potassium at 404.4 nm and 766.5 nm, are readily observed. The potassium line emissions have been investigated in the laboratory using premixed methane-air flames seeded with black liquor or potassium chloride solution mist. These laboratory investigations indicate that line emissions due to potassium at the two wavelengths (404.4 nm and 766.5 nm) can be used to calculate the gas temperature (assuming Boltzmann distribution) by the line intensity ratio technique. A 4-channel optical system has been developed, including a branched fiber-optic bundle, each branch being connected to a bandpass filter, photodetector, and amplifier. The system allows simultaneous measurements of intensities of the two potassium lines and the corresponding background (continuum) emissions. The four color system is interfaced with a personal computer equipped for simultaneous data acquisition on four channels. The four color system has been used successfully to measure gas temperature in potassium seeded premixed methane-air flames in the laboratory. However, as the combustion zone of a recovery boiler is large, with significant nonuniformities in temperature and concentration distributions, optical depth differences and self adsorption are likely to become prevalent. A cooled traversing probe has been designed and developed to investigate the reaction zone of a typical recovery boiler and to assess the effect of optical depth differences at the two wavelengths used in the line intensity ratio technique. In addition, these tests will provide data on the local heat flux in a black liquor recovery boiler reaction zone.

In addition to these tests, a prototype probe system is being assembled for testing at a paper mill site. Successful application of this technique to black liquor recovery boilers would demonstrate the technique's potential for use in other high temperature reactor systems.

Fundamental Studies of Black Liquor Combustion

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

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

A positive-displacement technique, in which individual droplets are extruded from a hollow needle, was developed earlier in this project for on-demand generation of highly viscous droplets with diameters of the order of 1 mm. This technique is now being used for injection of BL droplets (with up to 65% solids) into high-temperature streams in the DPFR. High-speed photography has been used for: (a) observation of the processes of BL droplet formation and detachment from the needle tip, (b) measurement of droplet diameters prior to detachment, (c) measurement of in-flight droplet diameters after detachment, and (d) velocities of droplets falling in a counterflowing hot gas stream. Droplet diameters in these studies can be varied from 1 to 2.5 mm, gas temperatures from 1000 to 1350 K, and gas velocities (upward) from 1.7 to 4.2 m/s. Studies in the auxiliary version of the DPFR, allowing droplet residence times up to about 0.6 s, have been completed. The full-height reactor offers the residence time capabilities of several seconds, depending mainly on the droplet diameter.

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

High-Temperature Oxidation of Chlorinated Hydrocarbons

A. Macek, N.O. Spears*, H.G. Semerjian

Control of products of incomplete combustion, generated during incineration of hazardous wastes, requires an understanding of rates and mechanisms of oxidation and thermal decomposition of its principal constituents (mainly chlorinated hydrocarbons). The experiments to provide such an understanding should be performed under well-controlled operating conditions which simulate full-scale incineration systems. A literature study has been made under the sponsorship of EPA, showing that at least three experimental research approaches should be considered: (a) laboratory burners or furnaces; (b) high-temperature flow reactors (providing they offer sufficient residence times for the reactant); and (c) fluidized beds. The first approach (flame destruction) is convenient, but it does not offer good control of three critical parameters for simulation of full-scale incineration systems: temperature, residence time, and oxygen concentration. Therefore, a decision has been made to explore the other two approaches.

A task on fluidized-bed destruction of hydrocarbons has been initiated. The existing NBS facility is being modified to allow: (a) the metering of gaseous reactants into the bed; (b) on-line exhaust monitoring of CO, CO_2, and possibly also O_2 and hydrocarbons, for determination of oxidation efficiency; and (c) extraction of gas samples for GC/MS analysis. Preparations are also being made to explore catalytic oxidation studies, for which fluidized-bed reactors are especially suitable. It is expected that the catalytic approach will offer a major advantage by allowing efficient oxidation at substantially lower temperatures than the corresponding gas-phase reactions.

Depending on the results of the fluidized-bed task, the dilute-phase plug flow reactor at NBS, which has just been constructed for droplet combustion studies, may be used for either gas-phase or droplet combustion of chlorinated hydrocarbons. The capability of attaining the desired temperatures (up to 1300 K), oxygen contents (0 to 21%), and gas residence times (1 s or more) -- as well as provisions for non-intrusive optical diagnostics -- are included in the basic design of the reactor. The flow capabilities of the reactor, and the droplet injection and observation capabilities, have already been demonstrated within the project on fundamentals of black liquor combustion.

*Howard University

Optical Measurements in Fluidized Bed Reactors

A. Macek, N.D. Amin

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

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

Fluorescence Spectroscopy for Control of Paper Pulping Processes

J.J. Horvath, H.G. Semerjian

There is an increasing need for the development of measurement science and technology for on-line measurement of process variables in the pulp and paper industry. Current process techniques for measurement of delignification rates in the pulping process are based on sampling and off-line analysis systems. The resultant delay prevents the on-line control of the digestor, and results in less than optimum operating conditions. The ideal process monitoring technique would be both an in-situ and real-time measurement system, so that important variables of the cooking process can be monitored and corrections applied before a cook is complete. The goal of this project is to develop in-situ techniques, based on fluorescence spectroscopy, for monitoring pulping processes.

In these studies, laser excited fluorescence of black liquor was investigated as a possible monitoring technique for pulping processes. A pulsed dye laser was used to examine the fluorescence spectrum of black liquor solutions. Various excitation wavelengths were used between 280 and 403 nm. Black liquor fluorescence spectra were found to vary with both excitation wavelength and black liquor concentration. Laser excited fluorescence was found to be a sensitive technique for measurement of black liquor with good detection limits and linear response over a large dynamic range. Measurements have recently been made on actual pulping liquors obtained from a paper mill. During the course of a 3 hour pulp cook, six and seven samples were obtained at various times from two separate runs. Laser excited fluorescence spectra were obtained, from these very optically dense liquors, using a backscatter configuration without any sample dilution. The fluorescence spectra obtained from these samples were found to vary during the cook, indicating good possibility of using fluorescence for a process control monitor. Future work will involve the study of cooking liquors from different type woods or from different stages of the paper making process.

PROCESS SENSING GROUP

Orifice Discharge Coefficient Database Development

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

A fully documented database has been developed for flange orifice meters. Two projects have been completed: Coefficients in the intermediate range of Reynolds numbers were obtained in the NBS-Gaithersburg water flow facility, while the high Reynolds number work was done in collaboration with an industrial gas pipeline company at their Joliet, IL, test facility.

As reported last year, the electroless nickel plating of all meter tubes prevented a continuous rust growth and thus, in turn, steady drift of orifice pressure drop measurements as observed previously. A set of fully reproducible data was obtained and subsequently submitted to the American Petroleum Institute (API).

The new data base, which will eventually replace the old one developed in the 1930's, was presented to the public in a joint API-GRI-NBS seminar in September 1986. This new database represents a major achievement and a new milestone in flow metrology. It will improve the accuracy of flow measurement and thus contribute to equity in the domestic and international trade of oil and gas.

IrO_2 Ionic Sensors

K.G. Kreider, S. Semancik

Reactively sputtered iridium oxide is being considered as a pH sensing material. It has the advantage that thin films could be fabricated inexpensively on probes which would be smaller and more durable than presently used glass electrodes. The IrO_2 is not attacked at high temperatures and pH levels which would destroy the glass electrode. We have produced reactively sputtered iridium oxide pH sensing films on Al_2O_3 substrates. We have found the temperature of the deposition affects the crystalline structure of the films and their electrical resistivity. The amorphous and crystalline films investigation was reported in J. Vac. Sci. Technol.

Although linear Nernstian behavior (59 mV/pH) has been observed in all of the sputtered films, a drift of the zero pH voltage (E.) appears to vary with fabrication conditions and exposure to air and solutions. We have systematically varied the activity of the H_2O during exposure by baking and autoclaving and are relating the variation of (E.) to what may be hydroxylation. Photoemission spectroscopy is being used to characterize the effect of fabrication variables and exposure on the composition of the surface of the IrO_2.

Following our report to the Nuclear Regulatory Commission (NRC) on "Review of Materials for pH Sensing for Nuclear Waste Containment" we are initiating a five year project to investigate the use of IrO_2 pH sensors in monitoring high temperature brines. The intent of the investigation is to enable the NRC to make accurate long range predictions of the corrosion of nuclear waste containment vessels.

Thin Film Thermocouples for Heat Engines

K.G. Kreider

The goal of this project is to demonstrate the feasibility of a materials system and fabrication technique for measuring temperatures inside the combustion chamber of ceramic insulated engines using thin film thermocouples. The ceramic insulating materials under investigation include partially stabilized zirconia (PSZ) in both monolithic and plasma sprayed forms and alumina (Al_2O_3). The thermocouple systems have included type E (chromel-constantan), type N (nisil-nicrosil), and platinum-platinum (with 6% rhodium). Adhesion studies for these systems indicate that a reactive metal bond coat such as Cr or Ti is very useful in insuring a strong (70 MPa) bond between Pt and PSZ or Al_2O_3. Scanning electron microscopy and electron microprobe analysis have indicated that the sputtered films were produced with the same composition as the target alloys, and continuous, strong, pore-free deposits can be sputtered 1-4 μm thick. Calibration, high temperature exposure, and flame testing of the sputtered thin film deposits indicate that a sputtered Al_2O_3 film is necessary for the type N thin film thermocouples and advisable for the Pt-Rh thermocouples if they are to be used for long times above 900 K. Because of the sensitivity to the atmosphere and alloy changes by diffusion of the thin films, type E thermocouples are unstable at 1000 K and are not recommended.

Humidity Sensing Employing Bifunctional Polymer Membranes

P.H. Huang

The electrical and thermodynamic characteristics of water vapor adsorption/desorption on a bifunctional polymer membrane have been investigated for humidity sensing at high levels of relative humidities and elevated temperatures above 50°C. The membrane is a thin film of hygroscopic, fluorinated organic polymer having pendant functional groups of a relatively strong sulfonic acid type and groups of a relatively weak carboxylic acid type. Electrical conductance of the thin membrane is measured as a function of relative humidity and temperature, using a frequency range of 100 Hz to 100 kHz. Based on the measured conductance data, values of differential thermodynamic functions of enthalpy and entropy are found to be significantly larger than those previously obtained for a sensor system at relative humidities and temperatures above 70 percent and 50°C, respectively. The thermodynamic data obtained are further used to characterize and interpret the phenomena of bonding states of water molecules and hysteresis ocurring in the sensor system. A patent application has been filed, based on the use of a bifunctional polymer membrane in humidity sensors.

Calibration Upgrade for Humidity

S. Hasegawa

The final test for the upgrade was the NBS gravimetric hygrometer vs. the NBS two-pressure humidity generator intercomparison test to verify the performance of the humidity generator. The results of the test verified that the generator was performing within the specified accuracy. The calibration documentation was completed and approved by the Calibration Advisory Group. The document is now going through NBS editorial review. Plans for a low frost point humidity calibration facility have been completed and the construction of the generator has been started. This facility will provide calibration services for moisture contents less than 1 ppm in selected gases.

Chemical Gas Sensors

S. Semancik, D.F. Cox, J.E. Erickson, T.B. Fryberger, K. Kreider

Tin oxide, SnO_2, has been used in a variety of solid state gas sensing applications because its conductivity is sensitive to the oxidation potential of its environment. We have conducted a model study on a (110) single crystal of this material in order to investigate the mechanisms by which these practical electrical changes develop. Although pure SnO_2 is a n-type semiconductor, having a band gap of 3.6 eV, we have demonstrated (using ultraviolet photoemission) that band gap defect states exist even for our single crystal specimen. These defects not only affect the electrical conductivity of SnO_2 in vacuum, but they are also important in gas adsorption processes, and therefore, help determine the conductivity changes produced in operating sensors.

Our efforts have been concentrated on correlating compositional (and structural) changes with changes measured in the surface conductivity of pure crystalline SnO_2. In-situ treatments have included adsorption from reducing and oxidizing gas backgrounds at 300 K and at elevated temperatures (which simulate actual operating conditions for certain SnO_2-based sensors). Analytical techniques utilized to determine the chemical and electronic properties of SnO_2 have included x-ray and UV photoemission, ion scattering, secondary-ion mass spectrometry, and in-situ 4-point resistivity measurements. In addition to providing fundamental insights into the operation and behavior of SnO_2-containing sensor devices, our work on SnO_2(110) has yielded an important baseline of results for work now underway on the effects of selectivity-enhancing metal additives in tin oxide.

We have also been studying a highly conductive oxide, indium tin oxide (ITO). This transparent oxide has the highest electrical conductivity of any transparent oxide and is useful in self heated windows. We have produced 2 μm thick films by reactive sputtering and are studying the adsorption-desorption of gas molecules on the surface of the ITO.

Standardized Chemical Measurement Methodology

Development and Laboratory Robotics

F.E. Jones

The work in this area has specific application to sensing, detection, collection, and analysis of selected chemical species in gases or deposited on surfaces. One of the objectives of this work is the optimization and standardization of methodology for the collection and analysis of volatile and semi-volatile organic compounds of interest. An annotated bibliography on collection and analysis of organic compounds in air has been prepared. The most prevalent methodology in this area (and, thus, is emphasized in the bibliography) is the collection and preconcentration of organic compounds in a tube or cartridge containing adsorbent (such as polymer beads) and subsequent desorption on to the column of a gas chromatograph (GC), GC-mass spectrometer (MS), or GC-MS-computer system for analysis. A robotic laboratory automation system has been ordered and delivery is expected in early FY 87. The system will be used to perform experiments on the analysis of gas samples, and on the analysis of contaminated and decontaminated surfaces. Interfacing of chemical sensors with the system and with a PC will also be investigated.

5. HONORS AND AWARDS

R.J. Santoro - Department of Commerce, Silver Medal Award for research on the fundamental processes leading to particle formation in high temperature chemically reacting flows, November 1985.

A. Macek - Department of Commerce, Bronze Medal Award for outstanding contributions to the science and technology of fluidized bed reactors, December 1985.

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Charagundla, S.R., Spectroscopic Temperature Measurement Technique for Recovery Boilers, DOE/Industry Advanced Sensor Working Group Meeting, Chicago, IL, Oct. 31, 1985.

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Cox, D.F. (coauthors: S. Semancik and P.D. Szuromi), Structural and Electronic Properties of Clean and Water-Dosed SnO_2(110), 32nd National Symposium of the American Vacuum Society, Houston, TX, Nov. 22, 1985.

Cox, D.F., H_2O Adsorption on SnO_2(110), Structural and Electronic Effects, Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA, Apr. 15, 1986.

Davis, R.W., Numerical Computation of Particle Trajectories: a Model Problem, AIAA/ASME 4th Fluid Mechanics, Plasma Dynamics, and Laser Dynamics Conference, Atlanta, GA, May 12, 1986.

Fryberger, T.B., Interaction of Boron with Mo(100) and its Effect on Surface Chemistry, Forty-Sixth Annual Conference on Physical Electronics, Austin, TX, June 17, 1986.

Gaigalas, A.K., Solid Fraction Measurement and Bubble Diagnostics, DOE/Industry Advanced Sensor Working Group Meeting, Gaithersburg, MD, Apr. 29, 1986.

Hasegawa, S., Hygrometry, Parameter Generation Control, Inc., Ashville, NC, May 5, 1986.

Horvath, J.J. (coauthor: H.G. Semerjian), Laser Excited Fluorescence Studies of Black Liquor, 1986 International SPIE Conference, Quebec City, Canada, June 6, 1986.

Horvath, J.J., Optical Diagnostics of Biomolecules, NBS Staff Research Seminar, NBS, Gaithersburg, MD, Sept. 5, 1986.

Horvath, J.J. (coauthor: H.G. Semerjian), LIF for Sensing in Bioreactors, 192nd National Meeting of the American Chemical Society, Anaheim, CA, Sept. 8, 1986.

Huang, P.H., Humidity Sensing Employing Bifunctional Polymer Membrane, The 2nd International Meeting on Chemical Sensors, Bordeaux, France, July 10, 1986.

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Kreider, K.G., Thin Film Thermocouples for Internal Combustion Engines,International Symposium on Metallurgical Thin Films, San Diego, CA, Apr. 9, 1986.

Kreider, K.G., IrO_2 Radio Frequency Sputtered Thin Film Properties, Solid State Transducers Workshop, Hilton Head, SC, June 6-8, 1986.

Kreider, K.G., Formation of Icosahedral Quasicrystals by Sputter Deposition, Annual Meeting of the AIME, Orlando, FL, Oct. 7, 1986.

Kreider, K.G., Thin Film Thermocouples for Temperature Measurement in Diesel Engine Cylinders, Automotive Technology Development, Contractors' Coordination Meeting, Dearborn, MI, Oct. 28, 1986.

Macek, A., Fundamentals of Black Liquor Combustion, DOE Black Liquor Research Program Review, University of Florida, Gainesville, FL, Feb. 19, 1986.

Macek, A. (coauthor: N. Amin), Solids Circulation in Fluidized-Bed Combustors, 21st Symp. (International) on Combustion, Munich, W. Germany, Aug. 7, 1986.

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Macek, A., Optical Diagnostics Inside Coal Combustors and Gasifiers, Brigham Young University, Provo, UT, Nov. 5, 1985.

Mattingly, G.E., NBS' New Slurry Flow Facility, Slurry Technology Association's Annual Meeting, Hilton Head, SC, Mar. 17-18, 1986.

Mattingly, G.E., Liquid Flow Measurement: Techniques for Metering, Calibrations, and Traceability, ASME Solar Energy Conference, Anaheim, CA, Apr. 14, 1986.

Mattingly, G.E., Gas Flow Measurement: Calibration Facilities and Fluid Metering Traceability at the National Bureau of Standards, Institute for Gas Technology Conference on Natural Gas Energy Measurement, Chicago, IL, May 1, 1986.

Mattingly, G.E., Vortex Shedding Flowmeter Research at NBS, Cranfield Institute of Technology Short Course Program, Cranfield, England, June 4-5, 1986.

Mattingly, G.E., LDV Measurements and Characterization of the Pipeflow Produced by the Notorious Elbows-out-of-Plane Configuration, Department of Mechanical Engineering Seminar, University of Surrey, Guildford, England, June 6, 1986.

Mattingly, G.E., Flowmeter Installation Effects: A New Approach to an Old But Prevalent Problem, International Conference on Flow Measurement in the 1980's, National Engineering Laboratory, East Kilbride, Scotland, June 10, 1986.

Mattingly, G.E., Gas Flow Measurement: Concepts, Facilities, and Traceability, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 15, 1986.

Mattingly, G.E., Specific Gas Flow Calibration Facilities at NBS-Gaithersburg, MD: Techniques and Performance Levels, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 15, 1986.

Mattingly, G.E., Fluid Flow Measurement: Concepts, Artifacts, and Implementation Techniques, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 16, 1986.

Mattingly, G.E., Numerical Modeling of Meter Flows: Orifice and Vortex Shedding Type, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 17,1986.

Mattingly, G.E., LDV Measurements of Vortex Shedding Flows, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 17, 1986.

Mattingly, G.E., Flowmeter Calibration Results - Techniques Recommended for Optimizing Performance, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 18, 1986.

Mattingly, G.E., Flowmeter Installation-Effects Research at NBS, DALFI's Advanced Gas Flow Measurement Course, Fort Collins, CO, July 18, 1986.

Mattingly, G.E., Industry-Government Consortium Programs on Fluid Metering Research, ASME/MFFCC Meeting, New York, NY, Sept. 11, 1986.

Mattingly, G.E., Fluid Flowrate Measurements: Techniques, Calibrations, and Traceability for Petrochemical and HVAC Applications, ISA Meeting, Wichita, KS, Sept. 22, 1986.

Mattingly, G.E., Two-Phase Fluid Jet Interactions, NBS-Nondestructive Evaluation Panel Presentation to NRC/NAS/NAE, Gaithersburg, MD, Nov. 21, 1985.

Presser, C. (coauthors: A.K. Gupta, R.J. Santoro and H.G. Semerjian), Velocity and Droplet Size Measurements in a Fuel Spray, AIAA 24th Aerospace Sciences Meeting, Reno, NV, Jan. 7, 1986.

Santoro, R.J. (coauthors: J.J. Horvath and H.G. Semerjian), Fuel Structure Effects on the Formation of Soot Particles in Laminar Diffusion Flames, Invited Review Paper, 60th Colloid and Surface Science Symposium, Georgia Institute of Technology, Atlanta, GA, June 15, 1986.

Santoro, R.J. (coauthor: H.G. Semerjian), Soot Formation in Diffusion Flames, AFOSR Contractors' Meeting, Stanford University, Stanford, CA, June 18, 1986.

Santoro, R.J., Soot Particle Formation Processes in Flames, Advanced Fuels Research, E. Hartford, CT, Oct. 4, 1985.

Santoro, R.J. (coauthors: T.T. Yeh, J.J. Horvath and H.G. Semerjian), The Transport and Growth of Soot Particles in Flames, Eastern States Section Meeting, The Combustion Institute, Philadelphia, PA, Nov. 4, 1985.

Santoro, R.J., The Formation, Growth and Transport of Soot Particles in Diffusion Flames, Mechanical Engineering Department, Louisiana State University, Baton Rouge, LA, Nov. 15, 1985.

Semancik, S. (coauthor: D.F. Cox), Experimental Studies of the Correlations Between Gas Sensor Response and Surface Chemistry, 32nd National Symposium of the American Vacuum Society, Houston, TX, Nov. 22, 1985.

Semancik, S. (coauthor: D.F. Cox), Fundamental Characterization of Clean and Gas-Dosed Tin Oxide, 2nd International Meeting on Chemical Sensors, Bordeaux, France, July 7, 1986.

Semancik, S., The Effects of Surface Additives on Gas-Metal Interactions, Institute for Physical and Theoretical Chemistry, University of Tubingen, Tubingen, West Germany, July 15, 1986.

Semancik, S., Temperature and Gas-Induced Property Changes at the Surface of Tin Oxide, Electronics Department, Technical University of Munich, Munich, West Germany, July 17, 1986.

Semerjian, H.G., Optical Diagnostics for Combustion Studies, University of Maryland, Department of Mechanical Engineering, College Park, MD, Apr. 4, 1986.

Semerjian, H.G., Particulate and Droplet Diagnostics in Spray Combustion, DOE/ECUT Working Group Meeting on Sprays, NBS, Gaithersburg, MD, Dec. 4, 1985.

Semerjian, H.G., Particulate and Droplet Diagnostics in Spray Combustion, DOE/ECUT Working Group Meeting on Sprays, Sandia National Laboratory, Livermore, CA, May 7, 1986.

Semerjian, H.G., Laser Tomography for Investigation of Turbulent Flames, AFOSR Contractors' Meeting, Stanford University, Stanford, CA, June 16, 1986.

Semerjian, H.G. (coauthors: C. Presser, A.K. Gupta and R.J. Santoro), Effect of Combustion Air Swirl on Liquid Fuel Spray Characteristics, 21st Symp. (International) on Combustion, Munich, W. Germany, Aug. 5, 1986.

Semerjian, H.G., Laser Tomography for Investigation of Chemically Reacting Flows, Institute for Paper Chemistry Seminar, Appleton, WI, Oct. 3, 1986.

Ulbrecht, J.J., Particle Transport Phenomena in Non-Newtonian Liquids, AIChE National Meeting, Miami, FL, Nov. 5, 1986.

Woo, S., A Practical Cooling Problem, Chemical Process Metrology Division Staff Seminar, NBS/CCE, Gaithersburg, MD, Oct. 15, 1985.

8. COMMITTEE MEMBERSHIPS AND EDITORSHIPS

COMMITTEE MEMBERSHIPS

G. Kulin

ASTM D.19 Main Committee on Water (Member)
- Task Group D19.03.03.02 on Velocity Measurements (Chairman)
- Task Group D19.03.03.03 on Velocity-Area Methods (Chairman)
- Task Group D19.03.03.08 on Measurement of Small Flows (Chairman)

G.E. Mattingly

ASME Main Committee on the Measurement of Fluid Flow in Closed Conduits (Member)
ASME SC-2 on Pressure Differential Devices (Member)
ASME SC-6 on Glossary of Terms for Flow Measurements (Member)
ASME SC-14 on Measurement of Fluid Flow Using Gravimetric and Volumetric Techniques (Chairman)

ASME SC-15 on Installation Requirements for Orifices, Venturis, and Nozzles (Member)
ASME SC-16 on Vortex Shedding Type Flowmeters (Member)
ASME Main Research Committee on Fluid Meters (Member)
ASME SC-11 on Test Methods and Calculation Procedures (Chairman)
ASME Ad Hoc Committee on Flowmeter Installation-Effects Research (Member)
International District Heating Association Fluid Metering Committee (Member)
ASHRAE Standards Committee 125P on Method of Testing Heat Meters Used in Fluid HVAC Systems (Member)

N.E. Mease

ASTM D0.22 on Methods of Sampling and Analysis of Atmospheres (Member)
ASTM D22.01 on Quality Control (Chairman)
ASTM SC.02 on Methods of Sampling and Analysis (Member)
ASTM SC.05 on Calibration (Member)
ASTM SC.11 on Meteorological Measurement (Member)

J.J. Ulbrecht

AIChE International Activities Committee (Member)
AIChE National Programs Committee, Subcommittee on Mixing (Member)

A.Macek

Combustion Institute - 21st Symposium (International) on Combustion, Program Subcommittee (Member)
NSF Panel on Presidential Young Investigators Awards (Member)

C. Presser

ASME K-6 Committee on Heat Transfer in Energy Systems (Member)

R.J. Santoro

Combustion Institute
21st Symposium (International) on Combustion
Program Subcommittee (Member)
Publications Committee (Member)
Eastern States Section - Papers Chairman

H.G. Semerjian

Combustion Institute - 21st Symposium (International) on Combustion - Program Subcommittee (Member)
ASME K-11 Committee on Heat Transfer in Fires and Combustion Systems (Member)
AIChE Engineering Sciences and Fundamentals Group, Area 1b - Kinetics, Catalysis and Reactor Engineering (Member)
AIChE Food, Pharmaceutical and Bioengineering Division, Area 15C - Biotechnology (Member)
NBS Research Advisory Committee (Chairman)

ASTM Subcommittee E29.04 on Characterization of Liquid Particles (Member)

EDITORSHIPS

J.J. Ulbrecht

Chemical Engineering: Concepts and Review, Gordon and Breach (Series Editor)

9. PROFESSIONAL INTERACTIONS

INDUSTRY

K.R. Benson

Cooperative research with R. Peele, Corning Glass Works, Corning, NY, on nitrogen flow by characterizing laminar meter performance as a transfer standard.

Cooperative research with P. Twigg, Westinghouse Electric Corporation, Baltimore, MD, on the accuracy of laminar flow with nitrogen for AWAC aircraft.

G.E. Mattingly

Instigated and coordinated NBS acceptance, installation, and check-out of Flowmeter Calibration Facility donated by Flow Technology, Inc., Phoenix, AZ.

Convened progress review meetings of Industry-Government Consortium on Vortex Shedding Stability to review NBS research results at NBS, Gaithersburg, MD.

N.E. Mease

Cooperative calibration work with J.D. Crosby, Belfort Instrument Co., Baltimore, MD, on anemometers to be used in automated, voice-activated, airport weather stations.

S.R. Charagundla

Collaboration with P. Ariessohn, Weyerhaeuser Co., Tacoma, WA, on emission measurements in recovery boilers.

Cooperative work with R. Kimball, Weyerhaeuser Mills, Plymouth, NC, on recovery boiler measurements.

J.J. Horvath

Collaborative research with C. Ipock and P. Farmer, Weyerhaeuser Co., New Bern, NC, on measurements for paper pulping processes.

A. Macek

Cooperative work with R. Corbeels, Texaco Research, Beacon, NY, on combustion of coke particles in fluidized beds.

A. Macek and H.G. Semerjian

Collaboration with E. McHale and M. King, Atlantic Research Corp., Alexandria, VA, on slurry combustion.

C. Presser and H.G. Semerjian

Collaborative research with W. Bachalo, Aerometrics, Inc., Mountain View, CA, on droplet size measurements in sprays and spray flames.

Collaborative research with D. Holve, Insitec, Inc., Danville, CA, on droplet size measurements in sprays and spray flames.

R.J. Santoro and H.G. Semerjian

Collaboration with P. Solomon, Advanced Fuel Research, E. Hartford, CT, on temperature measurements in diffusion flames.

H.G. Semerjian and S.R. Ray

Collaboration with P. Solomon, Advanced Fuel Research, E. Hartford, CT, on laser tomography.

S. Semancik

Collaborative work with R. Schaeffer, Extrel Corporation, on mass spectrometer modifications.

ACADEME, NATIONAL LABORATORIES AND GOVERNMENT

G.E. Mattingly

Research liaison with I. Anderson, Naval Research Lab, Washington, DC, on metal atomization research.

Coordination with C.W. Reimann, NBS National Measurement Laboratory, Gaithersburg, MD, on flow measurement standards strategies in the ISA and NCSL.

Coordination with W. Callis, U.S. Air Force, Newark, OH; J. Miller, U.S. Army, Huntsville, AL; and M. Gee and R. Chessman, U.S. Navy, Pomona, CA, on specific steps to initiate realistic traceability for fluid flow measurements.

N.E. Mease

Cooperative calibration work with a visiting scientist from the People's Republic of China on Pitot-static tube rake to be used for his measurements at Boeing in Philadelphia, PA.

Collaborative research with E. Simiu of the NBS Center for Building Technology, Gaithersburg, MD, on measurements to specify wind-based aeroelastic loadings on structures.

B. Robertson

Collaboration with C. Deslouis and B. Tribollet, Physique des Liquides et Electrochimie, l'Universite Pierre et Marie Curie, Paris, France, on electrochemical measurement of diffusivity.

S.R. Charagundla

Collaborative effort being developed with B. Northram, NASA Langley Research Center, Hampton, VA, on fiber optics sensing techniques.

R.W. Davis

Collaborative research with H. Baum, NBS Center for Fire Research, Gaithersburg, MD, on numerical modeling of chemically reacting flows.

Collaborative research with R.J. Santoro, Pennsylvania State University, State College, PA, on the physical aspects of diffusion flame modeling.

Collaborative research with W.M. Roquemore, Air Force Wright Aeronautical Laboratories, Dayton, OH, on the physical aspects of diffusion flame modeling.

Cooperative research with W.M. Pitts, NBS Center for Fire Research, Gaithersburg, MD, on the dynamics of coflowing propane-air jets.

J.J. Horvath

Collaborative research with J.L. Katz and D. Chin, Johns Hopkins University, Baltimore, MD, on absorption and fluorescence measurements in counterflow diffusion flames.

A. Macek

Collaborative research with W. Liggett, NBS Center for Applied Mathematics, Gaithersburg, MD, on statistical analysis of mixing processes in fluidizing beds.

Collaborative research being developed with D. Smoot, Brigham Young University, Chemical Engineering Department, Provo, UT, on diagnostics in entrained flow gasifiers.

C. Presser

Cooperative research with T. Lettierri, NBS Center for Manufacturing Engineering, Gaithersburg, MD, on calibration of particle sizing techniques with polystyrene spheres.

C. Presser and H.G. Semerjian

Collaborative research with A. Gupta, University of Maryland, College Park, MD, on diagnostics in spray flames.

Collaborative research with H. Hayasaka, Hokkaido University, Japan, on radiation modeling for reacting flows.

S.R. Ray and H.G. Semerjian

Collaborative research with R. Goulard, George Washington University, Washington, DC, on laser tomography.

R.J. Santoro and H.G. Semerjian

Cooperative research with R.A. Dobbins, Brown University, Providence, RI, on interpretation of optical measurements of particles in flames.

Collaborative research with K. Smyth and W.G. Mallard, NBS Center for Fire Research, Gaithersburg, MD, on particle formation in high temperature reacting flows.

Cooperative research with D. Santavicca, Pennsylvania State University, State College, PA, on Raman temperature measurements in particle laden flames.

Cooperative research with J. Katz, Johns Hopkins University Baltimore, MD, on temperature and particle measurements in high temperature reacting flows.

H.G. Semerjian

Collaborative research being developed with J. Gentry, University of Maryland, College Park, MD, on investigation of levitated droplets.

Collaborative research with V. Hlavacek, State University of New York, Buffalo, NY, on heterogeneous reactions and chemical vapor deposition.

Collaborative research with S. Sikdar, NBS Center for Chemical Engineering, Boulder, CO, on concentration measurements in bio-separation systems.

Collaborative research being developed with T. McAvoy, University of Maryland, College Park, MD, on pattern recognition and algorithmic sensors.

H.G. Semerjian and J.J. Horvath

Collaborative research being developed with A.E. Humphrey, K.P. Brown and J. Phillips, Lehigh University, Bethlehem, PA, on optical sensing in bioreactors.

H.G. Semerjian and A. Macek

Cooperative research with D. Clay, Institute of Paper Chemistry, Appleton, WI, on black liquor combustion and pyrolysis.

Cooperative research being developed with I. Stockel, University of Maine, Orono, ME, on droplet formation and black liquor combustion.

Collaborative research with R. Chawla, Howard University, Washington, DC, on combustion of hazardous wastes.

H.G. Semerjian and C. Presser

Cooperative work with J. Bellan and M. Clayton, JPL, Pasadena, CA, on diagnostics and modeling in spray combustion.

Cooperative research with D. Butler, Los Alamos Scientific Laboratories, Los Alamos, NM, on modeling of spray flames.

Cooperative research with J. Greenberg and Y. Tambour, Technion-Israel Institute of Technology, Haifa, Israel, on modeling of fuel spray dynamics.

Collaborative research with S. Ridder, F. Biancaniello and J. Manning, NBS Institute for Materials Science and Engineering, Gaithersburg, MD, on liquid metal atomization.

J.W. Erickson

Collaborative work with C.D. Olson, NBS Institute for Materials Science and Engineering, Gaithersburg, MD, on energy dispersive x-ray characterization of tin oxide.

Collaborative work with P.J. Estrup, Department of Chemistry, Brown University, on kinetics and thermodynamics of surface processes.

T.B. Fryberger

Collaboration with P.C. Stair, Department of Chemistry, Northwestern University, on the effects of adsorbed boron on the surface chemistry of molybdenum.

S. Semancik

Collaborations with R. Helbig, Applied Physics Department, Universitat Erlangen, West Germany, on the study of tin oxide single crystals.

Collaboration with D.L. Doering, Department of Physics, University of Florida, on structural and chemical effects of alkalis on metal surfaces.

Collaboration with T.E. Madey, NBS Center for Chemical Physics, Gaithersburg, MD, on surface coadsorption interactions.

10. CONFERENCES, WORKSHOPS, AND SEMINARS

CONFERENCES

Session on Soot at the Eastern Section Meeting of the Combustion Institute, Philadelphia, PA, Nov. 4, 1985. Chaired by R.J. Santoro.

Session on Combustion Diagnostics at the 24th AIAA Aerospace Sciences Meeting, Reno, NV, Jan. 7, 1986. Organized and chaired by H.G. Semerjian.

Session on Combustion Generated Pollutants at the 21st Symposium (International) on Combustion, Munich, W. Germany, Aug. 6, 1986. Chaired by H.G. Semerjian.

Session on Combustion of Solid Propellants at the 21st Symposium (International) on Combustion, Munich, W. Germany, Aug. 8, 1986. Chaired by A. Macek.

WORKSHOPS

Hosted workshop of DOE/ECUT Spray Working Group, held on Dec. 4, 1985 at NBS, Gaithersburg, MD. Organized by H.G. Semerjian.

Hosted Workshop on Biochemical Measurements, held on Apr. 17, 1986 at NBS, Gaithersburg, MD. Organized by J.J. Ulbrecht.

NBS-DoD Calibration Coordination Group Workshop to develop tailored fluid flow measurement traceability program, held on Aug. 19, 1986 at NBS, Gaithersburg, MD. Hosted by G.E. Mattingly.

NBS-U.S. Industry Representatives Workshop to explore possibilities to initiate an automated metal atomization consortium research program, held on Oct. 31, 1986 at NBS, Gaithersburg, MD. Contributory hosts: G.E. Mattingly and H.G. Semerjian.

SEMINARS

A. Szilvassy, Office of International Relations, National Office of Measures, Budapest, Hungary: Flow Measurement Activities of the National Office of Measures - Budapest, Hungary, Oct. 9, 1985.

M.H. Kim, Chemical Engineering Department, Northwestern University, Evanston, IL: Theories for the Flow of a Suspension and Comparisons with Experimental Data, Dec. 6, 1985.

K.C. Muck, Guest Scientist, NBS Center for Fire Research, Gaithersburg, MD: Complex Turbulent Boundary Layers, Mar. 14, 1986.

W.H. Schwarz and T.S. Margulies, Department of Chemical Engineering, Johns Hopkins University, Baltimore, MD: Acoustic Wave Propagation in Non-Newtonian and Multiphase Fluids, June 18, 1986.

I.P. Castro, Department of Mechanical Engineering, University of Surrey, Guildford, U.K.: A "Wall Stress Sensor" and its Use and Performance in Fluid Mechanics Research at the University of Surrey, Aug. 21, 1986.

W.D. Bachalo, Aerometrics, Inc., Mountain View, CA: Simultaneous Measurements of Drop Size and Velocity Distributions in Sprays, Oct. 11, 1985.

R. Prudhomme, Princeton University, Princeton, NJ: Dispersion of Liquids, Oct. 15, 1985.

F. Beretta, University of Naples, Naples, Italy: Ensemble Laser Light Scattering Technique for the Analysis of Atomization of Coal-Water Slurries, Oct. 29, 1985.

C. Jensen, University of Minnesota, Minneapolis, MN: Reactors for Chemical Vapor Deposition, Nov. 22, 1985.

D.J. Holve, INSITEC, Danville, CA: Development and Applications of Non-Intrusive Instrumentation for Particle Measurements, Dec. 5, 1985.

Tse-Wei Wang, University of Tennessee, Chemical Engineering Dept., Knoxville, TN: Applying Modern Control Techniques to Bacterial Growth Systems, Jan. 21, 1986.

M. Zachariah, University of California at Los Angeles, Chemical Engineering Dept., Los Angeles, CA: Experimental and Numerical Studies of Sulfur Chemistry in Flames, Mar. 13, 1986.

R. Sonntag, ARCO Oil Co., Plano, TX: Breakup of Latex Aggregates in a Shear Field, Apr. 16, 1986.

A. Vranos, United Technologies Research Laboratory, E. Hartford, CT: Planar Imaging in Cross-Flow Jets and Diffusion Flames, May 13, 1986.

M.M. Sharma, University of Bombay, Dept. of Chemical Technology, Matunga, Bombay, India: Excursions into Multiphase Reactions, May 19, 1986.

J.L. Katz, Johns Hopkins University, Baltimore, MD: Nucleation-Homogeneous, Photo-induced, of SiO_2 and Others, June 3, 1986.

A. Babchin, Electrochemical Technology, Inc., Seattle, WA: Modeling of Heat and Mass Transfer, June 25, 1986.

A. Schmidt-Ott, Laboratorium fur Festkorperphysik, Zurich, Switzerland: Aerosol Photoemission, July 23, 1986.

J.O.L. Wendt, University of Arizona, Chemical Engineering Dept., Tucson, AZ: Coal Pyrolysis in Flat, Laminar, Opposed Jet Combustion Configurations, July 25, 1986.

P. Lipowicz, University of California at Berkeley, Dept. of Chemical Engineering, Berkeley, CA: Aerosol Characterization of a Smoldering Source, July 29, 1986.

A. Garo, CNRS, Mulhouse, France: Oxidation of Soot Particles in a Laminar Diffusion Flame, Sept. 12, 1986.

M. Allen, Stanford University, Dept. of Mechanical Engineering, Stanford, CA: Digital Imaging Techniques in Reacting Flow Fields, Sept. 16, 1986.

D. Dunn-Rankin, Sandia National Laboratories, Livermore, CA: Particle Size Distribution Development During Pulverized Coal Combustion, Sept. 22, 1986.

A.V. Hamza, Department of Chemical Engineering, Stanford University, Stanford, CA: The Activation of Alkanes on Ni (100), Jan. 2, 1986.

J.D. DeNuzzio, Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA: Conduction and Stability in Ammonium/Hydronium B^{11} - Alumina, Feb. 4, 1986.

D.S. Simons, NBS Center for Analytical Chemistry, Gaithersburg, MD: Overview of Secondary Ion Mass Spectromety, Apr. 17, 1986.

Y.W. Chung, Department of Materials Science and Engineering, Northwestern University, Evanston, IL: Surface Chemical Modification by Titanium and Manganese Oxide, Sept. 10, 1986.

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Technical research activities performed by the Center for Chemical Engineering during the Fiscal Year 1986 are summarized herein. These activities fall within the general categories of process measurement, thermophysical properties data, and chemical engineering science. They embody: development and improvement of measurement principles, measurement standards, and calibration services such as volumetric and mass flow rates, liquid volume, liquid density, and humidity; generation (via accurate measurement and advanced predictive models) of reliable reference data for thermophysical properties of pure fluids, fluid mixtures, and solids of vital interest to industry; and development of improved correlations, models, and measurement techniques for complex flows, heat and mass transport, mixing, and chemically reacting flows of interest in modern unit operations.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

calibrations; chemical engineering; data; fluid mechanics; fluid properties; process measurement; research; sensors; solid properties; thermophysics; unit operations.

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