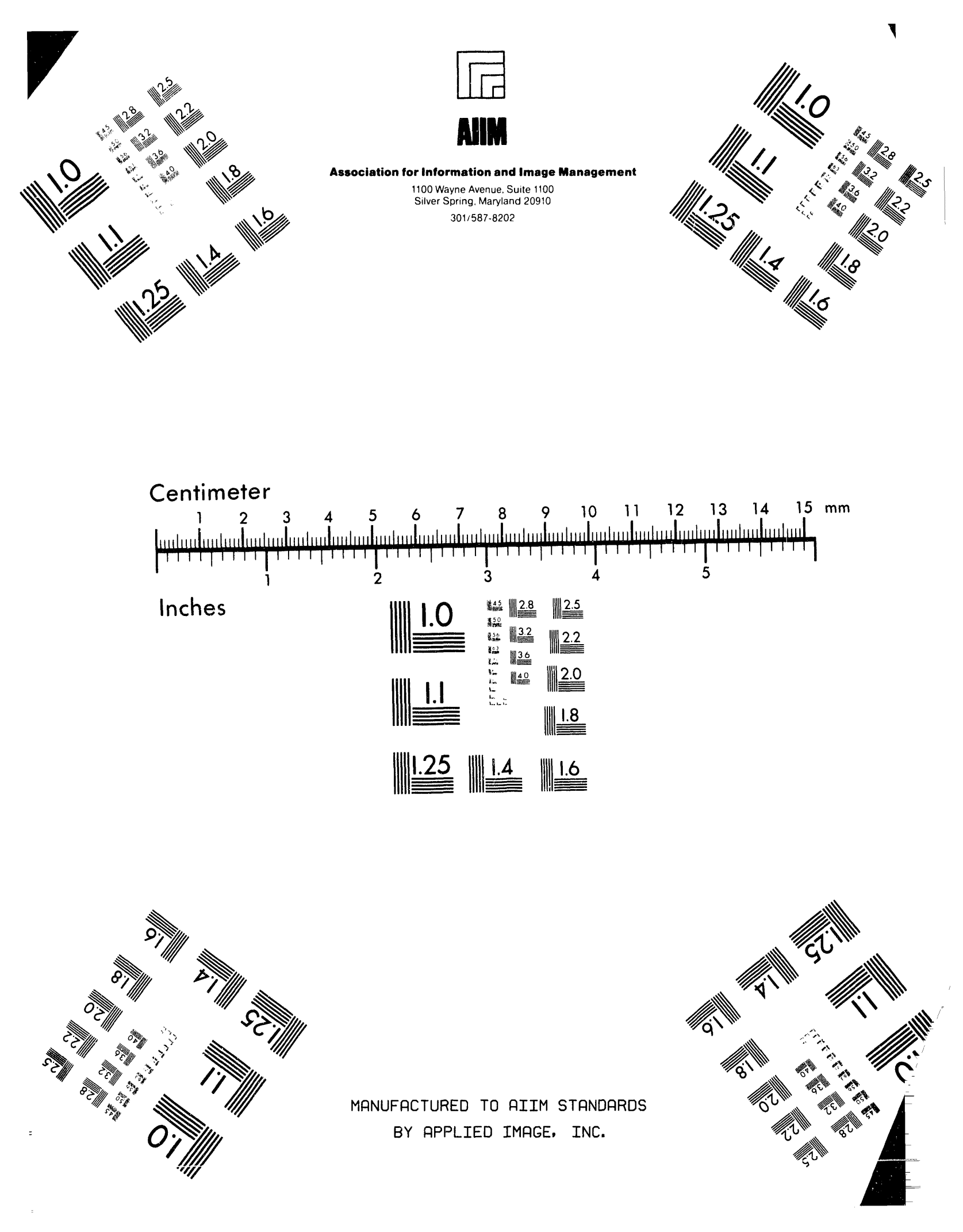
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DOE/OSTI--11633/4
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May 1993

Office of Industrial Technologies Research in Progress

U.S. Department of Energy
Office of Energy Efficiency
and Renewable Energy
Office of Industrial Technologies

This report was compiled for the Office of Industrial Technologies from project summaries contained in the Research-In-Progress (RIP) database of the Office of Scientific and Technical Information, Oak Ridge, Tennessee. The RIP database describes new and ongoing energy and energy-related research projects carried out or sponsored by the Department of Energy.

Contents

PROGRAM OVERVIEW

The U.S. Department of Energy (DOE) Office of Industrial Technologies (OIT) conducts research and development activities which focus on improving energy efficiency and providing for fuel flexibility within U.S. industry in the area of industrial conservation. The mission of OIT is to increase the utilization of existing energy-efficient equipment and to find and promote new, cost-effective ways for industrial facilities to improve their energy efficiency and minimize waste products.

To ensure advancement of the technological leadership of the United States and to improve the competitiveness of American industrial products in world markets, OIT works closely with industrial partners, the staffs of the national laboratories, and universities to identify research and development needs and to solve technological challenges.

DOE has signed more than one hundred Cooperative Research and Development Agreements (CRADAs) which combine the research capabilities of the national laboratories and the commercialization potential of U.S. businesses. In addition, OIT-supported projects are typically funded on a cost-shared basis with the private sector. To date, OIT has supported more than three hundred research and development projects; many of these efforts have helped implement energy-efficiency improvements in a variety of industrial applications.

To encourage industrial implementation of energy-conserving technologies, research and development efforts are supplemented with a variety of technology transfer activities and information exchanges.

This report contains summaries of the currently active projects supported by the Office of Industrial Technologies.

Deputy Assistant Secretary
Office of Industrial Technologies

INDUSTRIAL ENERGY EFFICIENCY

Advanced Heat Exchangers

Babcock & Wilcox Company
Lynchburg, VA 24506
R and D Division

1. *R & D of a Ceramic Fiber Composite Heat Exchanger*

Barringer, E.A.

This project is in the last phase of a three-phase effort. Phase I involved (1) determining the technical and economic feasibility of an advanced material (ceramic fiber reinforced ceramics) heat exchanger; (2) identifying critical problems relating to development of the heat exchanger; and (3) identifying and detailing Phase II R & D required for the successful design, fabrication, and operation of the critical components. Phase II consisted of (1) R & D to solve the critical problems and (2) completing the final conceptual design. Phase III consists of detailed design and construction of a test module, and its installation and testing in an industrial waste stream. The heat exchanger is designed for efficient and economic recovery of waste heat from major industrial high-temperature (589 °C) corrosive–fouling gas streams existing in steel soaking pits, aluminum remelt, and glass melting operations. An industrial user has been selected and will provide a consulting role to provide user perspective of the work.

Oak Ridge National Laboratory
Oak Ridge, TN 37831
Metals and Ceramics Division

2. *Ceramic Materials Support*

Karnitz, M.A.

This project provides materials technology support to the Industrial Energy Efficiency Division of the Office of Industrial Technologies and their contractors in two general categories: (1) high-pressure heat exchange system (HiPHES) and Advanced Heat Exchanger project support and (2) technology development. Project support involves assistance to Department of Energy (DOE) contractors in the development of systems for improved process heat exchange and for recovery of waste heat from industrial processes. The operating conditions of these systems require qualification of metallic alloys and ceramics for critical components such as heat exchanger tubes, seals, and structural members. The purpose of the project is to identify materials problems that significantly affect performance and reliability and to resolve the problems by application of existing materials technology or by performing the analyses and tests required for material qualification. The technology development portion of this project is focused on materials and processes that enhance industrial acceptance of ceramic and ceramic composite heat exchangers. The cost, performance, and reliability of ceramic materials and components are critical to the overall cost-effectiveness of both current systems and advanced concepts. The objective of this project is to develop improved materials and processes to overcome factors that increase cost (e.g., component fabrication) or that limit performance and reliability (e.g., corrosion and toughness).

Rensselaer Polytechnic Institute
Troy, NY 12180
Department of Mechanical Engineering, Aeronautical Engineering & Mechanics

3. *Enhanced Shell-and-Tube Heat Exchangers for the Industry*

Bergles, A.E.

The project objective is to evaluate enhancement of boiling heat transfer on the outside of tubes. It will address (1) the scaleup of shell-side boiling from a single enhanced tube to a tube bundle, (2) the fouling of the enhanced surfaces, and (3) the enhanced shell-side boiling with multicomponent fluids. Rensselaer Polytechnic Institute (RPI) is progressing with single-tube testing, and the construction of apparatuses for bundle test and fouling tests. After completing single-tube testing, final selection of enhanced surfaces for use in bundle testing will be made.

Solar Turbines, Inc.
San Diego, CA 92138
Research-Advanced Technology

4. *Development of High-Pressure Heat Exchange Systems (HiPHES)*

Ward, M.E.

The project objective is to develop a high-pressure heat exchange system (HiPHES) based on ceramics. The HiPHES should be capable of transferring heat to air at high temperature (900 °C) and high pressure (1035 kPa), feeding an indirectly fired gas turbine. The heating source in the air heater will be provided by the exhaust gases from a municipal or hazardous waste incinerator. This will allow higher temperature operation of the gas turbine without introducing corrosive species into the turbine. An industrial host site for field testing was selected. Work is continuing on the preliminary design of both the indirectly fired gas turbine and heat exchange systems for the HiPHES. Material samples are being exposed to the exhaust of a hazardous waste incinerator.

Stone and Webster Engineering Corp.
Boston, MA 02210

5. *Development of High-Pressure Heat Exchange Systems (HiPHES)*
Williams, J.J.

The project objective is to develop an advanced high-pressure heat exchange system (HiPHES) for a convective steam reformer integrated with a directly fired gas turbine cycle. The HiPHES steam reformer is a catalyst-filled turbular reactor that produces hydrogen at elevated pressures for subsequent processing to methanol or ammonia. The HiPHES system should allow reaction temperatures 160 C higher than the current state of the art. A high pressure, combustible atmosphere furnace has been designed and fabricated to test candidate materials under a simulated reformer environment. Results of this testing will help determine the materials used for constructing the tubular portion of the design.

Continuous Fiber Ceramic Composites

Allied-Signal Aerospace Company
Torrance, CA 90501
Garrett Ceramic Components

6. *CFCC Applications for Diesel Engine Valve Guides*
Yeh, H.C.

The objective of this project is to develop a component fabricated of continuous fiber ceramic composite (CFCC) for a specific industrial application, that of low heat rejection diesel engine exhaust valve guides. The CFCC material will be a continuous carbon fiber-reinforced silicon nitride. The composite will be fabricated by slurry infiltration and densified by nitridation, sintering, or glass encapsulation hot isostatic pressing. This effort will include criteria determination, economic assessment, performance targets, and component and system design. An experimental proof-of-concept (POC) will be performed involving refining the processing, and screening candidate materials for their friction, wear, oxidation and corrosion resistance, and mechanical properties.

Alzeta Corporation
Santa Clara, CA 95054

7. *CFCC Radiant Burner Assessment*
Sullivan, J.D.

Continuous fiber ceramic composite (CFCC) radiant burners are being developed for use in residential and industrial applications to increase thermal efficiency, provide more uniform and controllable heat transfer to the process, and reduce emissions of nitrogen oxides and carbon monoxide. During the initial phase of the program, specific combustion applications will be identified that could benefit from the use of CFCC burner components. Thermal and structural modeling and testing, which are specific to the targeted combustion applications, will be performed. Results of the modeling and testing will be used to determine material costs and performance requirements.

Amercom, Inc.
Chatsworth, CA 91311

8. *Chemical Vapor Infiltration of Silicon Carbide*
Bird, J.O.

Chemical vapor infiltration (CVI) is a thermochemical process for producing a condensed phase through the reaction of a volatile precursor on a surface. CVI has demonstrated the near-net-shape fabrication of large, thermally efficient structures, difficult to fabricate using conventional means, with a variety of refractory carbide, nitride, oxide, and boride matrices. The objective of this project is to use silicon carbide as the base matrix material, reinforcing it with carbide, nitride, or oxide fibers. Current efforts are focused on (1) obtaining a nonoxidizing fiber–matrix interface to ensure the appropriate thermal and mechanical behavior of the composite; (2) developing a cold tooling process to tool the component at temperatures less than 500 C during the initial densification process; (3) obtaining graded matrix composites that incorporate both silicon carbide and alumina or mullite oxide materials to improve the chemical compatibility; and (4) producing controlled porosity preforms to withstand temperature and other stresses, and filter undesirable particulates at very low pressure drops.

Babcock & Wilcox Company
Lynchburg, VA 24506
Lynchburg Research Center

9. *Research and Development of Advanced Ceramic Materials/Processing Methods*
Long, W.G.

The objective of this project is focused on two liquid-to-solid-based processing methods, sol–gel impregnation and liquid infiltration, for developing advanced ceramic composite materials. These approaches should be ideal for the oxide-based composite system, since it will allow scaling to cost-effective manufacturing operations. Efforts will focus on various fiber coatings to obtain optimal interfaces between the fibers and the ceramic matrix. To fabricate near-net-shape products, filament-wound, sol–gel impregnated tubes will be produced. Additionally, alternate impregnation materials and components will be tested, and models developed to demonstrate the properties and reliability of continuous fiber ceramic composites (CFCCs) to manufacturers and end-users. Assessments of several high-temperature, energy-intensive industrial applications will also be performed.

Dow Chemical Company
Midland, MI 48674
Advanced Ceramics Laboratory

10. *CFCCs for Chemical Processing Applications*

Magley, D.J.

The objective of this project is to develop continuous fiber ceramic composites (CFCCs) for use in energy, chemical production, and waste incineration processes. A fiber-reinforced, self-reinforced silicon nitride material will be used to formulate the CFCC through tape casting. Tape casting is a technique whereby ceramic powders and organic binders are mixed and cast into thin sheets that can be laminated together to form a desired shape. After removing the organic binders, the laminated shape can be densified using conventional techniques to form a dense article. An assessment of the energy savings and reduced emissions as well as an energy impact evaluation and economic study of the manufacturing processes will be performed.

Dow Corning Corporation
Midland, MI 48686

11. *Polymer Impregnation and Pyrolysis (PIP)*

Gaul, J.H.

The first year objectives of this effort are (1) to assess industrial applications for continuous fiber ceramic composites (CFCCs), (2) to demonstrate the feasibility of fabricating 2-D composites using PIP processing, (3) to investigate alternate fiber chemistries to improve the existing materials base, and (4) to understand the mechanical failures of CFCCs. In PIP processing, the matrix polymer is first impregnated into the fiber architecture and cured by conventional heating methods. The composite is then pyrolyzed to temperatures greater than 1000 °C, which converts the preceramic matrix polymer to a porous ceramic. The composite is reimpregnated with the preceramic polymer, and pyrolyzed a second time. This step is repeated until the composite reaches the desired density. Four applications have been identified for evaluation: (1) gas turbine combustion liners; (2) gas turbine blades, vanes, and blisks (bladed discs); (3) high-pressure heat exchangers; and (4) atmospheric heat exchangers.

DuPont Fibers
Wilmington, DE 19880
Experiment Station 302

12. *CFCC for Heat-Management Equipment*

Weddell, J.K.

The goal of this project is to improve efficiency and reduce pollution in several energy-intensive applications such as waste heat recovery in power generation systems and high-temperature industrial chemical processes. This goal will be pursued by developing and incorporating chemical vapor infiltration (CVI) silicon carbide continuous fiber composites into these systems. Current efforts will focus on (1) assessing which energy-intensive applications will benefit from the use of continuous fiber ceramic composite (CFCC) components, (2) assessing the performance and economic targets for those applications, (3) assessing the best fiber, preform, and oxidation protection systems for these composites, and (4) fabricating and testing the CFCC materials to provide a proof-of-concept (POC) for the selected applications.

DuPont Lanxide Composites, Inc.
Newark, DE 19714

13. *Directed Metal Oxidation Processing of Ceramic Composite Materials*

Rocazella, M.A.

The objective of this project is to develop ceramic materials through the novel DIMOX™ (directed metal oxidation) process for application in coal-fired combined-cycle power generating systems, steam reforming, and gas turbine systems. Two fiber-matrix composite systems will be evaluated. A silicon carbide fiber-reinforced alumina matrix composite will be evaluated for applications that require good thermal shock resistance, high fracture toughness, and excellent elevated temperature stability. Three types of silicon carbide fibers will be investigated with this system. Continuous Nicalon™ fibers will be evaluated in the form of 2-D braided fiber architectures. Chopped Nicalon™ fibers will be evaluated for applications demanding complex shapes, but low cost preform manufacture and hybrid fiber architectures will be evaluated for application requiring specific engineering properties such as high temperature strength and toughness. An aluminum oxide fiber-reinforced alumina matrix system will also be evaluated primarily for application where exceptional hot corrosion, aqueous corrosion, and oxidation resistance are required. The oxide fibers that will be evaluated with this system are the Almax™ alumina 2-D woven and 2-D braided fibers architectures.

General Electric Co.
Schenectady, NY 12301
Corporate Research and Development Center

14. *Toughened Silcomp Ceramic Composite*

Luthra, K.L.

The purpose of this project is to (1) demonstrate Toughened Silcomp technology, using a finer diameter fiber; (2) investigate and develop new preform fabrication techniques; (3) develop improved fiber coatings; (4) evaluate and optimize matrix microstructure; and (5) analyze the design and benefits of using continuous fiber reinforced composites for gas turbine components. Toughened Silcomp consists of silicon carbide fibers reinforcing a silicon–silicon carbide matrix, through melt infiltration processing. Molten silicon is put into contact with a heated preform of a carbonaceous material surrounding the reinforcing fibers, producing a matrix with a continuous network of silicon carbide. Toughened Silcomp will be

demonstrated in combustor and turbine tip shroud applications. These continuous fiber ceramic composites (CFCCs) have higher temperature capabilities compared to superalloys, and will reduce cooling requirements, allowing the turbine to operate with increased cycle efficiency, reduced fuel consumption, and/or increased power output.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

15. *Continuous Fiber Ceramic Composites: Supporting Technologies*
Karnitz, M.A.

The objective of this project is to study the fundamentals of materials, interactions, and failure analysis. Specific tasks will focus on (1) composite design: developing micro- and macromechanical models that predict the properties and behavior of composite components; (2) materials characterization: determining the effects of typical processing and service environments on composite materials; (3) test methods: ensuring quality control in characterizing, processing, and quantifying continuous fiber ceramic composite (CFCC) materials, using acceptable techniques and sensors to describe and measure their properties; and (4) life prediction and database development: understanding time-dependent behavior, environmental stresses, and damage accumulation that can limit the life of CFCCs, and compiling a database to collect and summarize data for all the tasks.

Textron Specialty Materials
Lowell, MA 01851

16. *CFCC Processing and Manufacturing*
Thomson, B.N.

The objective of this project is to develop and demonstrate processing methods for the fabrication of continuous fiber ceramic composites (CFCCs) for use in commercial and industrial applications. The end objective is to manufacture low-cost, ceramic composite tubes that can be used to improve industrial energy efficiency and productivity. The processing approach will use various fibers reinforcing a nitride-bonded silicon carbide matrix to fabricate tubular structures that will be impregnated and coated by a unique process to enhance durability called rapid densification. These ceramic composite tubes will be targeted for a variety of applications, particularly in systems used for the recovery of waste heat and power generation. Specifically, their use has been projected for reformers, pyrolysis furnaces, immersion heaters, burners, and preheaters.

Industrial Combustion Equipment

Alzeta Corporation
Santa Clara, CA 95054

17. *Research Program for Advanced Combustion Systems; Advanced Radiant Combustion System*
Sullivan, J.

The objective of this project is to develop, test, and demonstrate an advanced gas-fired radiant combustion system for use in industrial manufacturing processes that require very high, controlled heat fluxes at elevated process temperatures (up to 1000 °C). The burner being developed will extend radiant burner use to higher temperature processes, such as those in the petrochemical and metals processing industries. The planned initial installation is in a hydrogen-steam-reforming process, in which hydrogen is manufactured from methane. The combination of high heat flux at a uniform temperature means that loads can be heated efficiently without being subjected to localized overheating that might produce tube burnout, fluid coking, or material nonuniformities. An added advantage is that the low peak burner temperatures minimize or eliminate thermal NO_x formation (<30 to 40 ppm), resulting in a more environmentally acceptable combustion process.

Babcock & Wilcox Company
Alliance, OH 44601
Research and Development Division

18. *Development and Evaluation of a Workpiece Temperature Analyzer for Industrial Furnaces*
Berthold, J.W.

The current industrial practice for controlling the operation of steel processing furnaces relies on measurements of furnace gas temperature and workpiece surface temperature. Knowledge of the workpiece bulk temperature would be more useful, but it can only be estimated. The goal of this project is to develop and demonstrate a workpiece temperature analyzer to obtain the bulk workpiece temperature. The analyzer relies on laser generation and laser interferometer detection of an ultrasound wave in the workpiece. The time of flight of the wave between two points of known distance can be used to determine the velocity of the wave. For a given material, the velocity of the wave will define the temperature and can be determined with a calibration curve. This project first delineated promising potential markets, identified applicable hardware, and conducted a proof-of-concept (POC) laboratory test. In subsequent testing, sound waves were initiated and detected in steel alloy samples at temperatures in excess of 1200 °C. Potential subsequent activities include the application of increased laser power and improved signal processing, followed by the development of a prototype and its demonstration at a host site. Target applications

for this analyzer are those very high temperature processes associated with steel making: continuous casting and reheat.

Energetics, Inc.
Columbia, MD 21045

19. *Program Plan Development for Industrial Heating Equipment Research*

Jain, R.

The Office of Industrial Technologies (OIT) report "Advanced Technology Options for Industrial Heating Equipment Research" was sent out on November 30, 1992, to over 90 executives and experts from heating equipment industry, universities, trade associations, and national laboratories. This report describes 16 options for R & D in combustion of primary and waste-derived fuels, furnace, heat transfer, and combustion process control, along with the proposed measures to develop a comprehensive program plan. The cover letter not only solicited reviewers' views on the technologies described in the report but also allowed reviewers to identify any new technology options that might rank high in their opinion. All reviews are expected to be in by the middle of February 1993 following which an analysis of these reviews must be made and used to determine the further direction that is most appropriate towards developing the program plan.

Office of Industrial Technologies
Washington, DC 20024

20. *Program Plan Development for Fundamental Research in Municipal Solid Waste and Plant Waste Combustion*

Jain, R.

The Office of Industrial Technologies (OIT) has completed an investigation on research in municipal solid waste (MSW) and plant waste combustion, and has produced a draft report. The investigation basically consisted of (1) collection of information on refuse-derived fuels preparation, direct combustion, on-site burning, gasification and pyrolysis and (2) discussions of potential improvement areas with private sector executives and government experts. The report concludes with the recommendations of general and specific technical improvement areas where further investigation through a workshop or joint meetings would define the fundamental work that is not only lacking and useful but also intended to contribute to the work of others.

Praxair
Tarrytown, NY 10591

21. *Oxygen Enriched Combustion System Performance Study*

Schroeder, R.W.

The objective of this project is to evaluate the energy savings, environmental benefits, and overall performance of a full-scale, online industrial glass furnace in which nominal 100% oxygen has replaced air as fuel oxidant. The expectations that the replacement of air with oxygen would cut fuel usage, eliminate the need for a checker recuperator system, and improve glass quality and sharply reduce emissions have been verified by a demonstration at Carr Lowery and by the permanent installation of an "oxy-fuel" firing system at Gallo Glass. At Gallo, liquid oxygen was supplied by truck for over one year until oxygen from the world's first commercial-scale vacuum-pressure swing absorption (VPSA) system was in production. VPSA is a cost-effective means of supplying oxygen to the container glass and fiberglass production facilities. Gallo Glass is so pleased with the benefits realized from oxy-fuel firing that it will convert all remaining glass furnaces at its facility, the nations largest container glass plant, to oxy-fuel firing. The Gallo conversion is merely one manifestation of a trend strongly taking hold in the glass industry. At year-end 1992, oxy-fuel firing was used on glass furnaces with an aggregated capacity of 726 thousand kg/day (800 tons/day) of glass. Within two years, oxy-fuel firing capacity is expected to increase by four-fold.

Sandia National Laboratories, Livermore
Livermore, CA 94550

22. *Thermal Swing Absorption Process for Oxygen Separation from Air*

Jain, R.

The objective of this research is to define the potential to use the Thermal Swing Absorption (TSA) Process for oxygen separation from air for the online generation of oxygen-enriched air for combustion. This research is based on the premises that certain chemical compounds or substrates are capable of selectively absorbing oxygen at one temperature and desorbing this oxygen at a different temperature. The project includes (1) conducting a literature review to delineate chemical compounds or substrates that will selectively absorb oxygen; (2) experimentally measuring oxygen and nitrogen solubilities, oxygen absorption and desorption rates, and life of a few selected chemicals; (3) designing, fabricating, and operating a bench-scale experimental unit to validate the concept, obtain preliminary absorption-desorption data, and understand the chemistry and engineering challenges; (4) designing, fabricating, and operating a laboratory-scale experimental unit with separated absorber and desorber columns to collect more real-time data on absorber and desorber performance, heat transfer effects, pumping performance, and sorbents' thermal stability; and (5) preliminary technical and economic assessments of the system. Work will follow at Sandia National Laboratory (SNL) to verify performance of the best oxygen absorbing solutions synthesized by the University of New Hampshire and make

techno-economic assessments of a full-scale system, as the basis for a full-scale development of the TSA system.

Stone and Webster Engineering Corp.
Boston, MA 02210

23. *Assessment of an Industrial Wet Oxidation System for Burning Waste and Low Grade Fuels*

Bettinger, J.A.

The project objective is to develop a system to oxidize aqueous industrial wastes under supercritical water conditions with a goal of recovering energy from this process in the form of electricity or steam. Small-scale experimentation has shown that "sticky" solids and corrosion of the unit's materials of construction were barriers to prolonged, continuous operation of this process. A 1893 L/day (500 gal/day) pilot plant based on Modar vessel reactor technology has been constructed and will be operated to demonstrate continuous solids removal, determine waste destruction efficiency, identify improved construction materials, and determine the potential for energy recovery. The applicability of supercritical water oxidation technology to chemical, pharmaceutical, hazardous, and food waste processing was evaluated at the start of this project. The evaluations showed that supercritical water oxidation of hazardous waste was environmentally and economically attractive. Subsequent project phases involve further scaleup and the identification of equipment needed to recover exportable energy.

Surface Combustion, Inc.
Maumee, OH 43537-0428

24. *Research Program for Advanced Combustion Systems Ferrous Scrap Preheating System*

Maseman, N.

Nearly 40% of U.S. steel production is from recycled scrap using electric arc furnaces (EAFs). If the scrap enters the EAF hot, more steel can be produced in less time at a reduced cost. The preheater being developed and demonstrated for this project uses low-valued scrap steel coated with cutting oils. This oily scrap is heated with a hot, inert gas in the same bucket used to load the EAF. The oil on the scrap volatilizes and is ducted to a unique combustion system called a rich fume reactor (RFR). In the RFR the oil vapor along with natural gas are burned to form the hot inert gas that is directed back to the oily scrap in the scrap bucket. All vapors are burned prior to leaving the system. Since the preheater operates independently of the EAF cycle, retrofit installation is practical and process scheduling is possible. This system will be installed and tested at a "mini-mill" host site in the Pittsburgh area.

25. *Development and Evaluation of a Workpiece Temperature Analyzer for Industrial Furnaces*

Schultz, T.J.

The objective of this project is to develop and demonstrate an instrument that is capable of measuring the internal (or bulk) temperature of workpieces during heat treatment. Key target markets are in nonferrous strip and plate, steel strip, continuous casting, and carburizing. Use of this instrument will reduce manufacturing cost through increased manufacturing efficiency, reduced energy consumption, scrap reduction, and improved product quality. The system uses a laser to induce an ultrasonic acoustic wave through the workpiece. The speed of the acoustic wave depends on the temperature and is calculated by determining the time-of-flight of the wave over the distance traveled through the workpiece. Arrival of the acoustic wave is detected by using a laser interferometer. The instrument measures the temperature of the workpiece itself, not the temperature of the gas surrounding the workpiece. A signal processing technique has also been developed that enables the detection of ultrasound through three inches or more of steel, aluminum, and brass at temperatures up to 1024 °C. Carbon steel phase changes have also been detected. The system has been unaffected by vibrations, heat, and dirt that are common in industrial environments. The next step is to construct a commercial size unit and conduct a demonstration at a target market host site.

Industrial Heat Pumps

Astronautics Corporation of America
Madison, WI 53716

26. *Development of a Magnetic Refrigerator for Liquefaction of Hydrogen*

Foster, R.

Magnetic refrigerators that do not use chlorofluorocarbons (CFCs) utilize the magneto-caloric effect whereby paramagnetic materials heat up when magnetized by a high-field superconducting magnet and cool down when demagnetized. By cycling the paramagnetic material in and out of the magnetic field a highly efficient refrigeration cycle can be achieved. The development of a magnetic refrigerator to liquefy a precooled hydrogen will be a four-phase effort planned to span six years. Phase I is for a final design of a subscale prototype, Phase II is for subscale prototype fabrication and development testing. Phase III is a full-scale design of a 907 kg/day (1 ton/day) hydrogen liquefier, and Phase IV is the fabrication and test evaluation of the liquefier.

Duke Power Company
Charlotte, NC 28242
Marketing and Rates Department

27. *Development and Test of Heat Pumps in New Applications for Industry*

Baston, B.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing the IHP, and Phase III encompasses field testing of the IHP.

Gulf States Utilities Co.
Beaumont, TX 77704

28. *Development and Test of Heat Pumps in New Applications for Industry*

Smith, R.C.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing the IHP, and Phase III encompasses field testing of the IHP. Efforts are currently focused on Phase II of the project. A proposal has been received and accepted for one industrial plant.

Linnhoff March, Inc.
Leesburg, VA 22075

29. *Development and Test of Heat Pumps in New Applications for Industry*

McMullan, A.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing the IHP, and Phase III encompasses field testing of the IHP. Efforts are currently focused on Phase II of the project. Two industrial plants are currently under review.

Litwin Engineers & Constructors, Inc.
Houston, TX 77079

30. *Development of Advanced Prototype Chemical Heat Pump for Industrial Application*

Halsell, C.M.

Litwin Engineers and Constructors, Inc. is working cooperatively with Energy Concepts Company to develop a liquid/vapor absorption chemical heat pump system that will be demonstrated at a host site to be determined. This chemical heat pump system will utilize the fluid Alkitrate™ that Energy Concepts has developed under Office of Industrial Technologies (OIT) support and with cooperation of Oak Ridge National Laboratory (ORNL).

Minnesota Mining and Mfg. Co.
St. Paul, MN 55144-1000

31. *Advanced Brayton Cycle Solvent Recovery Heat Pump*

Jain, N.

A third generation heat pump design is being developed to recover and recycle volatile organic compounds (VOCs) from industrial air or gas streams. This technology is an alternative and more economic means of controlling VOC emissions from industrial processes. Previous research has demonstrated the Brayton cycle heat pump (BCHP) capable of "shock cooling" solvent-laden air streams, thus allowing condensation and collection of these solvents. Preliminary economic analysis shows attractive paybacks. Current research involves improvement to the overall heat pump cycle efficiency and the reduction of the capital cost of large-scale systems, and the development of smaller capacity heat pump systems that will be marketable to small industrial solvent recovery applications. Specifically, some improvements to the BCHP that have been identified and are under review in the preliminary design phase are (1) an activated carbon solvent concentrator to reduce the turbomachinery size requirements and (2) the utilization of selective adsorption beds to remove water from the solvent gas stream and thus avoid heat exchanger frost-up problems.

Nuclear Consulting Services, Inc. (NUCON)
Columbus, OH 43229

32. *Advanced Brayton Cycle Solvent Recovery Heat Pump*

Kovach, J.L.

The objective of this project is to cost-effectively control volatile organic compound (VOC) emissions streams from industrial processes by capturing and recycling them back to reusable solvents in an energy efficient manner. This project will complete the design and fabrication of a 1500-SCFM mobile regeneration system on a truck. The mobilized system will supply hot inert nitrogen gas that will regenerate the adsorbent beds located at small to medium solvent user sites. The solvent laden nitrogen stream will then be returned to the truck and the Brayton

system will condense the solvents out of the nitrogen system. The 1500-SCFM mobile system is a follow-on to the small 250-SCFM mobile Brayton cycle solvent heat pump system that is currently under operation at AeroChem, Hickory Springs, Dolco Packaging, and High Shear. Field testing of the Brayton system will address the most important factors affecting its marketability, which are the system reliability and the quality, and thus value, of the solvents recovered from the system. These factors are critical in affecting the economics and levelized annual cost of any VOC recovery technology.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

33. *Chemical Heat Pumps*

Olszewski, M.

The objective of this work is to identify, develop, and encourage industrial adoption of chemical heat pump technology. By utilizing reject process heat as the primary energy source, this technology offers industry the potential for maximum fuel utilization with reduced emissions. The goals are to identify and evaluate heat pump concepts, develop systems through the proof-of-concept (POC) stage, and commercialize the technology through industrial partnerships. Primary emphasis is being given to high lift concepts that could potentially supply process heat, steam and/or (sorption) refrigeration to a central plant utility (rather than a unit process application). A program plan for this area is being developed and implemented through a combination of in-house and industrial contractor research.

Oklahoma Gas and Electric Co.
Oklahoma City, OK 73101

34. *Development and Test of Heat Pumps in New Applications for Industry*

Prasad, B.H.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing the IHP and Phase III encompasses field testing of the IHP. Efforts are currently focused on Phase II of the project, designing the isobutane column to improve the performance of the heat pump.

Rocky Research Corporation
Boulder City, NV 89005

35. *Development of Advanced Prototype Chemical Heat Pumps for Industrial Applications*

Kirol, L.D.

Rocky Research, working cooperatively with Standard Refrigeration, is presently developing a 1 mm Btu/h unit that will pump heat from −9 to 54 °C using their newly patented solid–vapor heat pump design. This heat pump will be a single stage design and will pump heat from a cold ammonia stream at −9 °C to a hot water supply at 54 °C. That is, it will service a cooling and heating load with the same heat pump. The unit will be demonstrated to the Billman Foods plant in Zeeland, Michigan.

TENSA Services
Houston, TX 77058

36. *Development and Test of Heat Pumps in New Applications for Industry*

Tripathi, P.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing an IHP, and Phase III encompasses field testing of the IHP. Efforts are currently focused on determining a new host site for an IHP.

Utah Power and Light Co.
Salt Lake City, UT 84104

37. *Development and Test of Heat Pumps in New Applications for Industry*

Drennan, G.B.

The project objective is to identify new and novel approaches of industrial heat pumping (IHP) over a wide cross-section of industry, and then demonstrate to industry the cost benefits of IHPs with working examples. The scope of this project is divided into three phases. Phase I assesses process designs of IHP retrofits in a number of select plants. Phase II comprises developing a detailed design and installing an IHP, and Phase III encompasses field testing of the IHP.

ADVANCED INDUSTRIAL COGENERATION

Topping Cycles

Argonne National Laboratory
Argonne, IL 60439

38. *Gravel Bed Combustor for Solid Fueled Gas Turbine*

Cole, R.; Jain, R.

This project will demonstrate that an Allison Model 250 gas turbine rated at 298 kilowatts can be powered directly by a gravel bed combustor using wood chips and crushed coal. Project objectives are (1) to design and construct the pressurized gravel bed combustor, control system, and fuel feed system; (2) to conduct combustion tests of the pressurized gravel bed combustor at 5 atm pressure and 200 °C air preheat (using a control valve instead of the turbine to control the combustor back pressure), and to measure combustor performance and ash characteristics (the fuel will be approximately 2 cm pine chips); and (3) to develop a computer model of the gravel bed combustor that will simulate the combustion rate as a function of fuel properties and air-flow rate, pressure, and temperature. This research will help to promote efficient industrial cogeneration of electricity and process heat without the use of fuel oil or natural gas. Since corrosion and erosion are inherent problems for this combustor, Argonne National Laboratory (ANL) will perform techno-economic assessment of the methods to remove ash and alkali compounds at the combustor exhaust and devise modified combustor design to alleviate the corrosion and erosion problems. ANL will also perform a comprehensive market analysis for the combustor in cooperation with the turbine industry.

Battelle Memorial Institute
Columbus, OH 43201

39. *Ceramic Catalysts for Gas Turbine Systems*

Anson, D.

The objective of this work is to examine new ceramic materials that act as both the substrate and active catalyst for gas turbine combustion systems. Laboratory work has shown NO_x emissions of less than 5 ppm are achievable. This work will concentrate on durable ceramics.

ERC, Inc.
Tullahoma, TN 37388

40. *Wheeling/Transmission Access for Cogenerated Power Study*

Tessmer, R.G., Jr.

The goal of this project is to determine the effects of increased wheeling of power opportunities for new and existing cogeneration facilities.

Innovative Steam Technologies
San Diego, CA 92123

41. *High Performance Steam Systems Development*

Duffy, T.E.

This project is developing an improved steam cycle to operate at 10,345 kilopascals, 816 °C steam turbine inlet temperatures. A high temperature heat recovery steam generator (HRSG) and new steam turbine have been designed for these conditions. The new system will produce 100% more power over conventional steam equipment for a given thermal load (27,216 kg/h). A subscale HRSG was tested for 500 hours with no measurable wear or corrosion; materials testing has gone 4000 hours with no wear or corrosion. A full-scale HRSG has been completed and is currently being instrumented for a 1000 hour factory test. In addition, a 4 MW steam turbine is under construction and will be factory tested in 1993. A field demonstration will be planned following successful factory testing.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

42. *Long-Term Testing of Ceramics for Gas Turbines*

Ferber, M.K.

The goal of this project is to provide creep and static fatigue data on commercial ceramics after 2,000–10,000 hour exposure to test conditions. This data will be incorporated into the design criteria for ceramic components by gas turbine manufacturers.

Santa Barbara Air Pollution Control District
Santa Barbara, CA 93102

43. *Low NO_x Combustor Demonstration*

Keller, E.

A consortium of natural-gas fired turbine users is developing an improved combustor for existing online gas turbines in Southern California's nonattainment area for

NO_x emissions. Allison Gas Turbines will develop a modified rich–lean combustor to replace current combustors on engines at a Chevron gas pumping site. Consortium members include San Diego Gas and Electric, Southern California Edison, GRI, DOE, and Chevron.

Solar Turbines, Inc.
San Diego, CA 92138
Research-Advanced Technology

44. Advanced Turbine Systems

This 10-year project is a joint DOE–Fossil Energy and Conservation Energy effort to develop the next generation gas turbine systems for utility and industrial use. The project goals include a 60% system efficiency for utility systems (15% improvement for industrial scale units), single digit NO_x emissions, and a 10% reduction in busbar costs of electricity. Initial design studies will be started in 1993.

45. Ceramic Components for Stationary Gas Turbines

Van Roode, M.

The objective of this work is to retrofit key ceramic components into existing commercial stationary engines for cogeneration service. The incorporation of three components—the combustor, first stage nozzle, and first stage blade—will provide a 93 °C increase in turbine inlet temperature, a 6% increase in efficiency, and a 25% boost in power output. The retrofitted engine will be a Centaur H with resulting output of 4.5 MW. Initial design studies will be conducted in 1993 with help from 12 subcontractors including seven ceramic suppliers. The project will culminate with a 4000 hour field demonstration at an ARCO Bakersfield cogeneration site.

INDUSTRIAL WASTES

Waste Reduction: Gaseous Wastes

Argonne National Laboratory
Argonne, IL 60439

46. *Hydrogen Sulfide Utilization*
Harkness, J.B.L.; Gorski, A.J.

The project objective is to investigate and develop a new concept for recovery of valuable hydrogen and sulfur from gas streams contaminated with hydrogen sulfide. This concept involves using a low-temperature, microwave-generated plasma to dissociate the hydrogen sulfide molecule into its elemental components. This process represents a significant improvement over the current hydrogen sulfide waste treatment technology that loses the hydrogen value as wastewater. The economic benefit of recovering hydrogen and sulfur in a relatively simple, integrated process amounts to a near-term energy savings of over 13 x 10^{15} J/yr (12 trillion Btu/yr). Longer-term savings could amount from 30 to 74 x 10^{15} J/yr (30 to 70 trillion Btu/yr). An added benefit of this process concept is its potential for decreasing sulfur emissions from the current hydrogen sulfide waste treatment technology. The project consists of (1) a laboratory effort to verify the technical feasibility of the concept, (2) a systems engineering effort to evaluate the economic potential of this concept, and (3) a technology transfer effort to facilitate industrial acceptance of the process. The laboratory effort will involve experimentally determining the specific energy required to dissociate hydrogen sulfide, as well as the degree of conversion. The engineering evaluation will prepare a detailed, commercial-scale process design and use this design as the basis for an economic evaluation and market study. This study will determine the process sensitivity to the specific energy of dissociation and conversion, and will evaluate alternative applications of the technology. The technology transfer effort established an industry working group to provide technical guidance and to maintain an industrial focus for the laboratory research and the systems engineering.

Dow Corning Corporation
Midland, MI 48687-0994
Silicon Research

47. *Silicon Oxide Utilization*
May, J.B.

The objective of this project is to demonstrate, on a pilot plant scale, the commercial viability of new closed-furnace technology for smelting silicon and silicon alloys. The new technology will save materials and energy, reduce costs to improve U.S. competitiveness, and eliminate emissions by converting from open furnaces to closed furnaces with fume (SiO) and offgas (75% CO and 20% H_2) recovery. Closed-furnace technology is expected to avoid the loss of about 25% of the input silicon and about 50% of the total input energy. Annual energy savings of about 12 to 17 x 10^{17} J/yr (86 x 10^{12} Btu/yr) are predicted for the year 2010. Off-gas heating value is about 10 to 12 kJ/m^3 (350 to 390 Btu/ft^3). The retrofit of existing furnaces and building of new facilities in the United States will save 9000 U.S. jobs and avoid $1.7 billion/year in imported silicon. Based on successful tests in a 0.2-MW miniscale furnace, two pilot-scale furnaces were built. A 6-MW closed furnace with a direct-current submerged-arc heat source was built as a test facility for precommercial demonstrations. An existing 1.2-MW direct-current closed furnace was modified to demonstrate the production of ferrosilicon from low-cost feedstock (waste taconite, and waste coke fines or coke breeze) fed through a hollow electrode. Optimization tests for the 6-MW closed-furnace silicon pilot plant will be finished during FY 93, and commercialization projections for the closed silicon furnace will be updated. The project will be completed with the publication of the final report in FY 94.

Membrane Technology & Research, Inc.
Menlo Park, CA 94025

48. *Membrane Vapor Recovery Systems*
Baker, R.W.

The objective of this project is to develop and implement a new method of removing condensible organic vapors from various gas streams arising from industrial and commercial processes. This method will permit substantial improvement in the efficiency of removing volatile organic compounds (VOCs) from industrial and commercial gas streams. The increased efficiency of the removal process will result in energy savings and a direct reduction in VOC discharges. There will also be a substantial cost benefit through the capture of expensive VOCs that would otherwise be lost to the producer. This in turn will result in additional energy savings through reduction in the total production requirement for VOCs. The major technological issue is the development of a membrane that will function effectively and reliably under moderately high differential pressure (10 to 20 atmospheres) which is common in industrial applications. The project is divided into three phases and is currently in Phase II. The first phase consisted of the development and preparation of high-pressure modules and the design of the demonstration system. Phase II consists mainly of fabrication of the modules and construction of the demonstration system, followed by evaluation of the system performance, and arrangement of host sites for the field demonstration. Phase III will consist of field demonstration tests at the industrial sites and evaluation of the results.

Minnesota Mining and Mfg. Co.
St. Paul, MN 55144-1000

49. *Dual Cure Solventless Coating Process*

Keipert, S.J.; Sridhar, K.

The objective of this project is the development and commercialization of dual cure (DC) photocatalyst systems for the production of solventless coatings from urethane-precursor–acrylate and epoxy–acrylate monomer compositions. Upon irradiation, new organometallic photocatalysts produce both free radicals and Lewis acidic species that cause monomer curing. This is the first practical radiation curing of polyurethanes directly from monomers. Annual energy savings of 1.6 x 10^{16} J/yr (1.5 x 10^{13} Btu/yr) are predicted for the year 2010. The physical properties of the coatings have been extensively characterized in laboratory tests, and found to be generally superior to either of the monomers alone. For example, the toughness of the epoxy–acrylate coatings was found to be more than twice that of the tougher component (epoxy) monomer. Catalyst production and coatings for metal substrates were scaled up while continuing formulation development and characterization. FY 92 activities included proof-of-principle tests, the selection and preparation of coatings test coupon and tape substrates, optimization of topcoat and primer coatings, and tape saturant formulations. In general, the coatings have cured well despite significant pigment loadings. Activities for FY 93 will include completing topcoat and primer qualification tests; optimizing topcoat and primer coating application and cure techniques; updating technical, energy, and economics performance projections; and completing the project with the publication of a final report.

New York State Energy Research and Development Authority
Albany, NY 12223
Industrial Efficiency Programs

50. *VOC Control Strategies*

Howansky, H.

The NICE^3 program, in cooperation with Niagara Mohawk Power, Carrier Corp., ChemSystems, and New York State, is developing an innovative approach to the development and transfer of information on volatile organic compounds (VOCs) minimization and recovery technologies throughout industry. This program will demonstrate a low-cost, energy-efficient recycling and control technology designed for small businesses and small applications. Many industries, including printing, chemicals, pharmaceutical, metal cleaning, and laundries, rely on the use of solvents at intermediate points in their production processes. In many processes, the solvent ends its cycle as a vapor contaminant in a warm air stream. Research will focus on the development of computer software that will identify optimal VOC control strategies for individual facilities, and demonstrate an energy efficient solvent-condensing system for the capture and recycling of VOCs. This program will introduce industry to a comprehensive, cost-effective, and energy-efficient waste minimization technique.

Texas A & M University
Texas Engineering Experiment Station
College Station, TX 77843
Department of Petroleum and Chemical Engineering

51. *Vapor–Liquid Equilibrium*

Bullin, J.A.

The objective of this project is to develop and implement a new method of measuring vapor–liquid equilibrium (VLE) data using Fourier transform infrared (FTIR) analysis. This method will permit substantial improvements in the efficiency of amine solvent systems used to remove hydrogen sulfide from industrial waste gas streams. The increased efficiency of the amine systems will in turn result in energy savings and a reduction in carbon monoxide, carbon dioxide, and nitrogen oxide discharges. Successful assembly and testing of the 14-cm gas transmittance cell, the 86-m multipass gas transmittance cell, and the liquid Circular Internal Reflectance cell have been completed. Component frequencies for IR calibration have been completed, the diethanolamine (DEA) VLE system components have been calibrated, the acid gas–water solubility data has been compared with literature data, and acid gas–DEA VLE measurements have been completed. During FY 93, a journal article describing the equipment and IR measurement technique will be submitted for publication, as will acid gas–DEA VLE measurements. The system limits for quantitative measurement will be determined and methyldiethanolamine (MDEA) solutions will be calibrated. Acid gas–MDEA VLE measurements will be completed and submitted for publication. VLE measurements on the MDEA–DEA amine system will also be started.

Western Reserve Manufacturing Company, Inc.
Lorain, OH 44055

52. *Electric Tundish*

Nielsen, W.D.

This project pertains to the substantial industry that performs continuous casting of barstock in certain copper alloys. Such alloys, which generally include toxic lead and nickel, are employed in the manufacturing of bearings, bushings, and other critical machinery parts. A superheated reservoir of molten alloy is maintained in a continuously heated holding furnace (tundish) during casting. These tundishes are currently heated exclusively by fuel gas or oil and are only 20% energy efficient. The National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program in cooperation with Western Reserve Manufacturing Company, Inc. and the Ohio Development Agency, is proposing a new energy efficient system that would heat the tundish by electric induction means instead of fossil fuel. Additionally, electric induction will substantially improve the current process by eliminating corrosive, polluting waste gases and making possible the casting of lead-free bronze and copper plumbing.

Waste Reduction: Liquid Wastes

Avery-Dennison
Painesville, OH 44077

53. *Ultraviolet Curing*

McKee, D.R.

The Avery-Dennison's Fasson Films Division manufactures pressure-sensitive labels with silicone-coated paper or plastic release liners (backing material behind the peel-off mailing label). In its current use, this process requires hazardous-waste-producing solvents necessary in the overall production of the liners. The National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, in cooperation with Avery-Dennison and the Ohio Development Agency, is developing a UV curing process. This technology will use UV light to cure the backing for adhesive labels, providing an alternative to solvents, reducing manufacturing costs, and saving substantial energy.

California Division of Water Resources
Sacramento, CA 94105

54. *Ultrasonic Dishwashing*

Pike, C.

Current dishwashing technology was developed in the late 1800s. Large volumes of water are heated to approximately 82 °C, caustic detergents are added, and this solution is pressure-jetted against dishes. A new process is being developed by the National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program in cooperation with the California Division of Water Resources and Ultrasonic Products, Inc. to reduce the current dishwashing temperature to 38 °C through the use of ultrasonic cleaning. This new technology uses transducers that convert electrical energy into mechanical energy. Cooler water can be used because the cleaning action is derived from microbubbles that implode on the surface of the item to be cleaned at a rate of 40,000 times per second. Implosion creates the mechanical scrubbing, cleaning action and is omnidirectional, which allows it to permeate into the interior of objects with no dead spots. A series of tests will be used to verify the efficiency and effectiveness of the process, with the final product targeted at all institutional-size dishwashers. Benefits include substantially reduced water and heat requirements.

FMC Corporation
Pasadena, TX 77507

55. *Methanol Recovery Process*

Pulawski, M.

As a result of increasing methanol prices and rising disposal costs, recovery and reuse of spent methanol through steam distillation is under investigation by the National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, Texas Water Commission, and FMC Corporation. Steam distillation injects steam directly into the distillation column preventing the buildup of undesirable quantities of hydrogen peroxide and metal cations. Current efforts have shown that recovering the spent methanol through steam distillation will allow over 90% of the volume of methanol now used to be recovered. Research is now focused on other industries that have methanol waste streams for technology transfer. A case study will also be written to provide technical assistance to industry. This project involves specialized controls on the distillation process to avoid the buildup of peroxide and metal-ion concentrations, which can cause explosions. FMC has started installing similar units at its other facilities, based on very favorable results of this project.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

56. *Solvent Reduction through Use of Supercritical Carbon Dioxide Cleaning*

Benson, R.; Maestas, G.; Spall, D.

The objective of this project is to address technical challenges to supercritical fluid (SCF) systems development that will lead directly to commercialization of viable SCF-based technology for precision cleaning applications. The goal is to find acceptable replacement cleaning agents for undesirable solvents such as ozone-depleting halons, chlorofluorocarbons, carbon tetrachloride, and other fully halogenated alkanes. This project is developing data on applicability and operating parameters for supercritical carbon dioxide as a cleaner. The advantage of supercritical carbon dioxide cleaning is that it will generate minimal waste, and the waste that is generated, if released, will not significantly alter the environment. The research will determine if the cleaning of the materials tested is adequate, economical, and the overall energy savings meet the criterion of 10^{15} J/yr (10^{12} Btu/yr). The research is performed in conjunction with industry so that the technology is exchanged as it is developed. Testing with laboratory-scale equipment with several types of extractors has begun. Data has been generated on the removal of specific contaminants, response of some materials to cleaning media, and methodology for cleanliness testing. A pilot-scale superscrub with recycle was ordered and built. Planned activities for FY 93 include continuing investigation of cleaning effectiveness, efficiency, economic studies of various parts, and beginning equipment scaleup. During FY 94 the study phase will be completed and technology transfer will be actively pursued.

New Jersey Department of Environmental Protection and Energy
Trenton, NJ 08625

57. *Ultrasonic Tank Cleaning*

Wittenberg, N.; Gabel, S.; Tucker, B.; Nichole, G.

Current cleaning processes for chemical tanks and drums use considerable thermal energy to reprocess cleaning solvents, simultaneously generating considerable amounts of

chemical waste. The National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, in cooperation with the New Jersey Department of Environmental Protection and DuPont-Merck Pharmaceutical Company, is developing an ultrasonic cleaning technology for tank cleaning that will eliminate solvents, chemical waste, and energy required to reprocess solvents. Energy savings are estimated at 118 billion J/yr (112 million Btu/yr). Ultrasonic tank cleaning has application to thousands of sites.

PPG Industries, Inc.
Allison Park, PA 15101
Department of Environmental Engineering and Control

58. *Reclaim and Reuse Wastewater*

Palchek, G.E.; Tinter, M.; Kolvalsky, D.A.

To insure quality of water-based coatings for the automobile industry, the processing equipment for the water-based products is frequently cleaned with water. This generates thousands of liters of wastewater, which is now being disposed of as hazardous waste by transport to a state-licensed incinerator. The National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, in cooperation with the Ohio State Department of Development and Pittsburgh Plate Glass (PPG), is investigating a process to clean paint rinse wastewater to the point where it can be reused in the system. Modifications are required both to the treatment process and the paint cleaner system to incorporate the recycle process. The reclaimed water contains impurities at a low enough concentration that it can be reused. The impurities actually increase the cleaning effectiveness of the system. Therefore the water can be piped from the holding tank back to various manufacturing areas for reuse. Current results have shown a substantial reduction in the volume of hazardous wastewater requiring disposal from 1.5 million L/yr to 75,000 L/yr.

Sandia National Laboratories, Albuquerque
Albuquerque, NM 98195

59. *Solvent Reduction through Use of Self-Cleaning Soldering Process*

Inman, R.

The objective of this program is to compare the capabilities of a new, no-clean soldering process with those of existing wave soldering processes. It will develop data to prove electronic military hardware produced on the new system is reliable, paving the way for military specification changes. This is important because approximately 50% of all electronic equipment is manufactured per military specifications, and many commercial manufacturers use these as de facto specs. The new no-clean soldering process utilized in this project eliminates the need for cleaning solvents by using a dilute adipic acid flux to remove oxidation prior to soldering, and a dilute formic acid in a nitrogen cover blanket to inhibit oxidation during soldering. The adipic acid is evaporated during soldering, and the formic acid is converted to carbon dioxide and water. Environmental conditioning and surface insulation resistance (SIR) tests of a number of test boards were completed, and boards were sent to Los Alamos National Laboratory (LANL) for surface failure analysis. The test results will be used to support changes in Mil-Spec 2000 to allow the new no-clean process to be used. Surface analysis and accelerated life tests were performed, and the assembly and soldering of all the boards used in all aspects of the testing was completed. Activities for FY 93 include finalizing the results of all tests and developing and publishing a final report that includes the optimization study.

Waste Reduction: Solid Wastes

AAP St. Marys
St. Marys, OH 45885

60. *On-Site Aluminum Recycling*

Kobayashi, F.

AAP St. Mary's makes cast aluminum automobile wheels from ingots for domestic and foreign automotive vehicles. Machining rough castings produces aluminum chips that are contaminated with cutting oils and coolant. Typically, the contaminated chips are trucked to an off-site recycler where the chips are cleaned and melted into ingot for shipment back to AAP. There is a high amount of waste byproduct, and a new technology is needed for stirring the molten aluminum during the recycling process. The National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, in cooperation with AAP St. Mary's and the Ohio Development Agency, is investigating a solution by separating the chips from the oil contaminants and reducing the use of machining coolant by 50%. On-site reclaiming of chips is estimated to provide a 50% reduction in energy usage because the aluminum will be melted once.

California Integrated Waste Management Board
Sacramento, CA 95826

61. *Forty Percent Recycled Paper*

Dunn, T.X.; Hart, G.A.

In response to growing concerns about the amount of waste being generated, the National Industrial Competitiveness through Energy, Environment, and Economics (NICE^3) program, in cooperation with the California Integrated Waste Management Board, has initiated demonstrations on how a typical paper product manufacturer can substitute 40% of its raw fiber requirements with post-consumer mixed paper waste, and that this mixed paper waste is equivalent in quality and production to virgin paper. This research is intended to verify the efficacy of the final product, with the product aimed at those industries that have not traditionally used recycled paper fibers, such as the roofing industry. The energy reduction savings of this technology has been estimated at 60%.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

62. *Electroplating Waste Minimization and Treatment for Energy Savings*

Benson, R.; Maestas, G.; Smith, B.F.; Sauer, N.N.

Technologies for the reduction of electroplating wastes will be evaluated for their potential to increase the effectiveness of energy utilization in manufacturing processes and to reduce the detrimental impact on the environment. Sludges derived from electroplating processes represent both a high level of metal contaminants and energy loss when those metals are sent to landfills and not recycled. Metal ions used in plating operations are currently discharged as waste. The goal is to separate and purify these metal ions to allow reentry of this former waste into the front end of the process as reagents. These steps will give rise to energy savings because of reduced raw materials, mining expenditures, metal pressing, transportation, sludge processing, and sludge disposal needs. This technology is expected to slow the increasing inventory of stored metal sludges, which are becoming a state and national liability.

Waste Materials Utilization and Conversion: Gaseous Wastes

Engineering Resources, Inc.
Fayetteville, AR 72703
Biomass Research Center

63. *Biological Conversion of Waste Gases into Acetic Acid*

Gaddy, J.L.; Ko, C.-W.

The objective of this project is to develop a biological system utilizing anaerobic bacteria to convert the CO, CO_2, and H_2 found in certain industrial waste gas streams into acetic acid, which is a valuable industrial product. The proposed system will capture these waste gases in low concentrations, which are not currently economical to capture using chemical or mechanical methods. This technology offers the potential to reduce energy consumption in manufacturing acetic acid while reducing the discharge to the atmosphere of waste gases. The technical and economic feasibility of the biological production of acetic acid from waste gases has been demonstrated, and the best bacterial culture for this conversion has been selected. The process has been defined and very favorable economics projected. To move this technology rapidly toward commercialization, a prototype demonstration will be conducted in FY 93 involving prototype design, prototype construction, prototype operation, process scaleup, and commercial design. During FY 94 operation of the prototype unit will be completed, a commercial facility will be designed, and construction of the first commercial unit will begin.

University of Pittsburgh
Pittsburgh, PA 15260

64. *Production of Bisphenol-A Polycarbonate Using Carbon Dioxide*

Beckman, E.J.

The goal of this project is to develop a method by which bisphenol-A polycarbonate (BAPC) can be produced using carbon dioxide. Production by this method lowers both energy requirements and safety and environmental costs because of the replacement of the currently used phosgene monomer and reduction of the required process temperature. The primary foci of the experimental work are the effects of carbon dioxide density (a function of temperature and pressure) and absolute temperature on the reduction rate of the nitrophenyl carbonate with bisphenol-A to form the polymer. Carbon dioxide insertion reactions using molybdenum and vanadium compounds will be studied, as well as the use of tin-based catalysts. Activities planned for FY 93 are the procurement and installation of high-pressure reactors and the evaluation of oxy-tin compounds and other oxy-metal compounds for low-temperature reaction with carbon dioxide.

Waste Materials Utilization and Conversion: Liquid Wastes

Pacific Northwest Laboratory
Richland, WA 99352

65. *Catalytic Conversion of Food Manufacturing Wastewaters to Methane*

Elliott, D.C.

The objective of this research is to advance the Thermochemical Environmental Energy System (TEES) concept. This includes (1) operation and evaluation testing of the 454-kg/day continuous reactor; (2) catalyst development and lifetime studies to solve the problems of physical deterioration of the fabricated catalyst pellet and the loss, over time, of the catalyst activity; and (3) technology transfer activities to identify additional, appropriate waste streams for early market development. TEES has the potential to help industry solve several energy and environmental needs. TEES is a unique thermocatalytic gasification concept that converts wet industrial and food processing waste to methane for use in existing boilers and carbon dioxide (for bottling, packaging, and other uses). The process can also provide cogeneration, wastewater treatment, and reduction in solid waste handling. TEES is distinctive in its application to the food processing industry, and no biological or thermal process exists that has the potential to provide the overall systems impact of TEES. Process research will be conducted in existing bench-scale batch and continuous-feed reactor systems to evaluate energy production and the destruction of organics contained in the wastewaters. A scaled-up reactor system will be operated to determine the effects of scaleup and to document the proof-of-engineering for the process. Further development of TEES is anticipated and will be cofunded by industrial partners, including construction of a cost-shared on-site demonstration unit.

Waste Materials Utilization and Conversion: Solid Wastes

Air Products and Chemicals, Inc.
Allentown, PA 18195

66. *Utilization of Waste Tires Using Novel Surface Modification Technology*

Bauman, B.D.

The project objective is to produce novel composite materials by combining surface-modified, ground waste rubber with numerous commercially available plastics. Commercial incentives driving incorporation of surface-modified ground rubber will be manufacturing cost reductions or property enhancements in the composite material. Potential savings of approximately 82 million joules (78,000 Btu) can be realized for every kilogram of surface-modified scrap rubber incorporated in polymer composite systems. Task 1 markets applications development. Several polyurethane and polysulfide products have been identified; several demonstrations and evaluation tests will be done. Task 2 consists of designing a pilot plant and reevaluating the energy and economics of the technology. Applications that can consume significant volumes of surface-modified rubber will be identified and developed. Several approaches will be used including in-house R & D, contract research, and provision of samples to prospective end users.

Argonne National Laboratory
Argonne, IL 60439

67. *Research for Increased Utilization of Scrap Metal: Removal of Impurities from Scrap Cast Aluminum*

Daniels, E.J.; Wolsky, A.M.

The objective of this project is to develop an effective technique for removing trace amounts of antimony from secondary aluminum to improve the achievable mechanical properties of aluminum castings produced with the addition of strontium. The antimony in the recycle stream comes from castings produced by European and Japanese founders and used in automobiles, some of which are imported. The first goal is to survey members of the Aluminum Recycling Association (ARA) to determine antimony concentrations in secondary aluminum supply. The second goal is to determine the effectiveness of calcium as a scavenger of antimony. If calcium is proven effective, it would probably provide the most cost-effective method for removing antimony, as calcium–aluminum master alloys are used by the industry for the production of certain types of secondary ingot. The third goal is the transfer of technology to founders and smelters, which will include the presentation of results at the spring meeting of the Technical Committee of the ARA and at the 97th Casting Congress of the American Foundrymen's Society (AFS).

68. *Research for Increased Utilization of Scrap Metal: Automotive Materials Recycling*

Daniels, E.J.; Wolsky, A.M.

The objective of this task is to maximize the energy benefits resulting from cost-effective recycling of automotive materials and components. The near-term objective is to develop technology to provide for the recycling of the constituents of auto shredder residue, whereas the long-term objective is to examine the opportunities for "Design for Disassembly" and Design for Recycling™. This task is cost-shared by the Institute of Scrap Recycling Industries and also forms the basis of a cost-shared Collaborative Research and Development Agreement (CRADA) with the Vehicle Recycling Partnership (VRP). The approach that will be taken in this program is (1) to identify and quantify all waste streams that result from the recycling of obsolete cars, (2) to determine the current impediments to recycling of those waste streams, (3) to examine options for minimizing those waste streams, and (4) to determine which of those options is most cost-effective, environmentally acceptable, and institutionally acceptable within the existing structure of the U.S. automotive recycling industry. Among the broad options that will be considered in this program to minimize the wastes associated with recycling obsolete cars are (1) development of technologies to increase the recyclability of waste materials for their material values, (2) development of techniques to increase the recyclability of components for their value as replacement parts, and (3) examination of materials and component design options to increase the recyclability of future automotive components (design for remanufacturing) and materials (design for recycling).

69. *Research for Increased Utilization of Scrap Metal: Recovery of Metals and Fluxes from Secondary Aluminum Smelter Salt Cake*

Daniels, E.J.; Wolsky, A.M.

The objective of this task is to develop cost-effective technology for recovery and recycling of the constituents of secondary aluminum smelter drosses, slags, and salt cakes. The development of this technology will result in a significant increase in the production of finished aluminum from recycled aluminum and a decrease in the production from primary ores, minimizing the energy consumption required for production. Secondary aluminum recycling has the potential to conserve more than 316 x 10^{15} J/yr (300 trillion Btu/yr) of primary energy that would be consumed if that metal were otherwise produced domestically. If the metal were imported instead, the value of the metal would increase the trade deficit by about $2 billion per year. Two possible technology alternatives will be developed. The first approach uses a solvent to precipitate the salts from the saturated brine solution, which then results in a water–solvent stream and a precipitated salt stream. The second approach focuses on minimizing the amount of water required and also converts the aluminum-oxide fraction of the salt cake to a material input for primary aluminum producers. This task is cost-shared by the Aluminum Recycling Association through a CRADA.

70. *Research for Increased Utilization of Scrap Metal: Removal of Lead from Brass and Bronze Scrap*

Daniels, E.J.; Wolsky, A.M.

The objective of this task is to develop technology that will provide for cost-effective removal of lead from high-lead-content scrap used for the production of brass and bronze ingot. Copper-based alloys, which are used by the foundry industry to produce plumbing fixtures, have typically contained about 6% lead. The continued use of recycled copper-based alloys could be threatened by anticipated regulations that may limit the lead content of plumbing fixtures. A technique that may reduce the lead content of lead-bearing scrap is liquation; however, it is unlikely that liquation would be completely effective in removing the lead from the metal. Complete and selective removal of the lead would likely require the addition of a fluxing agent that would form an insoluble lead compound, which could then be removed from the molten metal. Alternative separation techniques, such as electrochemical dissolution and chemical leaching, may also be feasible, depending on the form of the scrap and the nature of the lead contained within the scrap (e.g., surface coatings such as solder, lead in solid solution, or alloyed lead). Two central issues that must be examined are (1) the need for lead removal in the first place and (2) the implications of lead removal, should it be technically feasible to effect the selective removal of lead from lead-containing copper-based scrap. This task is cost-shared by the Brass and Bronze Environmental Research Corporation through a CRADA.

71. *Research for Increased Utilization of Scrap Metal: Systems Analysis of Recycling Opportunities*

Daniels, E.J.; Wolsky, A.M.

The objectives of this task are (1) to identify the opportunities for increased recycling of materials from other scrap sources, (2) to evaluate the energy impacts and economic benefits of increasing the level of metals and associated materials recycling in industry, (3) to define R & D requirements, (4) to conduct preliminary experiments, and (5) to coordinate the research of this program with the research efforts of other organizations such as the Vehicle Recycling Partnership as well as with the other research efforts of the Office of Industrial Technologies (OIT) and DOE which relate to scrap metal recycling. Future opportunities for increased recycling from potential sources include the recovery of plastics from packaging materials production, primary lead furnace slags, and the recovery of metals from "red mud".

MUNICIPAL SOLID WASTE

Municipal Solid Waste

Air Products and Chemicals, Inc.
Allentown, PA 18195

72. *Cocombustion of MSW and Sewage Sludge*
Shahani, G.

In recent years, municipal planners have had to respond to stricter regulations governing the handling and management of sewage sludge. With ocean dumping banned and landfill disposal limited, cities are seeking alternative ways to manage sewage sludge. This project is investigating the use of oxygen-enriched combustion as a method for improving the incineration of sewage sludge. Sewage sludge can be burned in facilities designed for municipal solid waste (MSW), but the kinetics of combustion require that the ratio of sludge to MSW remain low. Efforts are focused on doubling or tripling the sludge percentage by increasing the oxygen level in the combustion chamber from 21 to 25%. Results have shown that waste streams consisting of up to 10% sewage sludge can be burned successfully in MSW waste-to-energy combustion facilities.

Argonne National Laboratory
Argonne, IL 60439

73. *Landfill Gas Research*
Bogner, J.

Methane, as a source of energy, has been collected from landfills for a number of years. Landfill leachate is expected to play a key role in increasing the production of methane. The purpose of this project is to investigate the effect of landfill leachate on methane production and determine how methane gas migrates within a landfill. Leachate is being recycled in an attempt to reduce its toxicity and increase methane production. In addition, through investigations of the quantity of methane generated from the refuse, the methane storage trends in landfills, lateral migration, recovery efficiency, atmospheric discharge, and the effect of methanotrophic bacteria, a model can be developed that could be used to estimate methane balance and to help design improved methane recovery systems. Initial results have revealed that methane recovery systems are not 100% efficient and landfills may have detectable levels of methane migrating in subsurfaces and through the landfill cover.

74. *Cofiring Refuse-Derived Fuel Pellets and Coal in Power Plants*
Ohlsson, O.

One alternative to accumulating municipal solid waste (MSW) is converting the combustible components of the MSW stream into a fuel source that could replace fossil-fuel-based energy sources and reduce sulfur dioxide emissions. A cooperative research and development agreement (CRADA) with two national laboratories and three industrial partners has focused on this alternative by characterizing the effects of burning a combination of binder-enhanced densified refuse-derived fuel (b-d RDF) pellets and coal in a commercial-scale electrical generating facility. Pelletized b-d RDF has been successfully burned in coal combustors, but only in quantities of less than 3%. Current efforts focus on cofiring RDF in quantities up to 20%. Operating, technical, and economic viability data will be obtained to determine the near-term commercial use of b-d RDF. In addition to the research, the CRADA participants are identifying any barriers inhibiting the commercial implementation of this technology.

National Renewable Energy Laboratory
Golden, CO 80401

75. *High-Solids Content of Anaerobic Digestion of MSW*
Rivard, C.

Anaerobic digestion has been known to convert the biodegradable portion of municipal solid waste (MSW) into methane gas, but has not been implemented in MSW processing. Relatively large reactors and the low concentration of solids processed have inhibited the utilization of anaerobic digestion as a waste-reducing, fuel-producing option. The purpose of this project is to design, fabricate, and test an anaerobic digester (high-solids fermenter) for processing an MSW stream containing high concentrations of solids. Current efforts have shown that the high-solids fermenter can process up to 35% solids in the reactor, producing methane gas at seven times the rate of conventional systems. In addition, the system's innovative agitator design allows for extremely efficient mixing with low energy consumption. This can reduce the need for process liquids as well as reduce the size of the reactor.

76. *Anaerobic Digestion of Municipal Solid Waste and Tuna Sludge for American Samoa*
Rivard, C.

The purpose of this project is to apply anaerobic digestion techniques to a mixed waste stream of tuna sludge and municipal solid waste (MSW) on American Samoa. The sludge produced by the island's two tuna canneries and MSW produced by the population is creating a problem for MSW management. American Samoa prohibits extensive landfilling of MSW. In addition, the two canneries continue to dump tuna sludge a few miles off shore, an action that is environmentally controversial and expensive. Results have shown success in utilizing the high-solids fermenter to process the mixed solid waste stream in the laboratory. Current focus is on two related efforts that will lead to a pilot-scale demonstration on American Samoa. The first is evaluating the maximum process feed

rate for the anaerobic high-solids process and the second is designing and fabricating an intermediate-scale reactor with a 1000-L capacity.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

77. *Socioeconomic Factors Affecting Decisions on Waste-to-Energy Projects*

Curlee, T.R.

A startling number of planned waste-to-energy (WTE) facilities have been either delayed or canceled during the last five years. Oak Ridge National Laboratory is conducting research that will give waste planners a better understanding of the technical, social, and economic factors that contribute to the cancellation of planned WTE facilities. Current research is being conducted in two phases. In the first phase, numerous WTE projects throughout the United States will be examined. Data models will be used to determine the degree to which the various demographic factors influence the decision. The second phase utilizes a team of anthropologists, geographers, urban planners, and economists to investigate four communities that chose to implement or abandon WTE projects. Interviews and literature review will be conducted, and the influence of regulatory issues, financial considerations, the level of public involvement, community characteristics, and local environmental issues will be examined.

Solid Waste Association of North America
Silver Spring, MD 20910

78. *Evaluating Materials Recovery Facilities*

Frola, C.

Insufficient information exists on the energy consumption, economics, and environmental impacts associated with operating a materials recovery facility (MRF). The purpose of this project is to collect and analyze data on these factors so municipal planners, waste managers, and the scientific community can better assess MRFs as a waste management option. This research will give planners and administrators a better understanding of operating and maintenance expenses, the effect a facility will have on human health and the environment, and the role played by energy-driven activities (for example, transportation, lighting, heating, and plant processes). Current efforts are focused on assessing the economic, energy, and environmental aspects of six operating MRFs.

79. *Mercury and Dioxin in Waste Streams*

Shaub, W.; Voell, C.

The combustion of polyvinylchloride (PVC)- and mercury-containing products in waste-to-energy plants is believed by the general public to cause harmful emissions. Concerns exist about the formation of dioxins during the combustion of PVC and the hazards from mercury-containing household and hospital batteries that are burned with municipal solid waste (MSW). The purpose of this project entails compiling all the available information on the emission of chlorine compounds and mercury when MSW is combusted in waste-to-energy facilities. The relevant information collected will be made accessible to the scientific community and to the public.

Wheelabrator Environmental Systems, Inc.
Hampton, NY 03842

80. *Controlling Acid Gas Emissions from MSW Combustion Units*

Ganotis, C.

The purpose of this research is to determine if lime ($Ca(OH)_2$) and sodium bicarbonate ($NaHCO_3$) injections can be used to successfully neutralize acid gas emissions from waste-to-energy combustion facilities. Lime is commonly used to reduce acid emissions, but it does so at a 50% efficiency rate. Sodium bicarbonate is more efficient, but it is expensive and can discolor the stack plume. Using the two reagents in concert, called duel sorbent injection, increases their effectiveness, making the process economical and reducing the acid gas emissions to levels required by the 1990 Clean Air Act Amendments. Current efforts will be focused on the reagents and variables such as injection rates, injection locations, boiler loads, and furnace temperatures. The long-term goal will demonstrate whether dual sorbent injection technology is a viable and cost-effective alternative for reducing acid gas emissions from municipal solid waste (MSW) combustion facilities.

SOLAR INDUSTRIAL PROGRAM

Decontamination of Water

National Renewable Energy Laboratory
Golden, CO 80401

81. *Solar Detoxification of Water*
Williams, T.

There are almost 20,000 contaminated water sites nationally, with an associated treatment volume of 28 trillion L/year (7.5 trillion gal/year). Approximately one-fourth of these sites are located in high-solar insolation regions of the country. DOE is working to reduce the cost of solar detoxification and increase its efficiency. Field experiments during FY 92 at a superfund site in Livermore, California and the Tyndall Air Force Base near Panama City, Florida have shown the technical feasibility of using solar energy to destroy hazardous chemicals contaminating groundwater. Development of solar reactors has led to rapid cost reductions that put the solar technology within reach of existing remediation technologies (carbon adsorption and UV–oxidation). During FY 93 the program will cost share in the design of solar detoxification systems with industry. These designs will result in improvements in system operation, control, and safety. The designs will lead to cost-shared field experiments in FY 94 at industrial or remediation sites to show the effectiveness and economics of the process. In parallel with system development, catalyst development will continue at NREL and at a number of supporting universities. Improvements in the efficiency of the catalyst will enable the manufacturers to demonstrate near-competitive economics with other waste management techniques.

82. *Solar Detoxification of Soil*
Williams, T.

There are an estimated 662 billion kg (730 million tons) of soil needing detoxification. More than a third of this contaminated soil is located in areas of high solar insolation, providing a market opportunity for solar technology. All efforts in this area are directed to a Tri-Agency project that was initiated to pool the resources of the Army's Toxic and Hazardous Materials Agency (THAMA), Environmental Protection Agency (EPA), and DOE in demonstrating the concept at the Sierra Army Depot. Interest in the technology centers on the possibility, indicated by laboratory experiments, that the solar process may result in fewer products of incomplete combustion than does incineration. During FY 92, Pacific Northwest Laboratory (PNL) (under contract to the Army) completed a feasibility study that concluded that the development of solar detoxification systems could be justified on the basis of either expected cost reductions or performance improvements. During FY 93, DOE will assist THAMA in the design of a pilot-scale demonstration plant to be built at the Sierra Army Depot. The plant will be completed and operated during FY 94. Data will be analyzed and the results will be compared to other remediation technologies.

Industrial Processes

National Renewable Energy Laboratory
Golden, CO 80401

83. *Advanced Applications of Solar Energy*
Williams, T.

There are a large number of industrial processes that can be conducted using solar energy. The market for advanced materials, for example, is estimated to be $150 billion by the year 2000. Solar applications are being explored in the areas of materials production and processing. Applicable markets include aerospace, engines, electronics, optics, and manufacturing. The High Flux Solar Furnace at National Renewable Energy Laboratory (NREL) was designed and built to push the frontiers of solar understanding. This furnace, based on an optical concept developed by the University of Chicago, has a unique capability for concentrating the sun's energy. It can produce a solar beam with the energy density found on the surface of the sun. It thus provides the program with an exceptional tool for finding new uses of solar energy. The furnace was first used to determine if solar energy could be used in materials processing. This work attracted industrial interest and resulted in Cooperative Research and Development Agreements (CRADAs) with Coors Ceramics and Brush–Wellman during FY 92. The primary objective of this activity during FY 93 will be to establish the feasibility of using solar energy to beneficially alter the properties of materials. This effort will center on the two CRADAs: the one with Coors to develop a new low-cost process for making silicon carbide, and the one with Brush–Wellman to develop a method for joining metal to ceramics. These efforts will produce pilot-scale demonstrations of the processes at the industrial sites in FY 94.

84. *Solar Process Heat*
Williams, T.

During FY 92, DOE conducted a survey of the states to determine the extent of interest in solar process heat. It was found that over 20 states were not only interested, but had funds available to cost share in solar industrial projects. This interest was tempered, however, by the need for information on the capabilities of the technology, including energy output and the cost of operating systems. To obtain this information, the program is cooperating with states to help them determine the potential of solar thermal energy and assisting the solar industry in initiating projects. During FY 91 and FY 92, the program funded prefeasibility studies to help solar companies and potential end users develop solar heating projects. These efforts resulted in more than 20 projects being initiated that turned $160 thousand funding into $1.6 million in solar projects. Technical assistance is provided to the solar industry through the Sandia Design Assistance Center. Discussions with state energy offices and military bases

during FY 92 will lead to more cost-shared solar projects in FY 93. These projects will supply the data needed by potential users to establish that the economics and energy output from solar process heat systems can be accurately predicted and that they can be reliably maintained. A database will be developed and kept updated to provide system performance information to all potential users of the technology. The program will work closely with the financial community to reduce the barriers associated with insurance and third party ownership.

COMBUSTION

Engine Combustion Technology

Drexel University
Philadelphia, PA 19104
Department of Mechanical Engineering and Mechanics

85. *Hydrocarbon Oxidation Chemistry*
Cernansky, N.P.; Miller, D.; Robinson, F.

Drexel University has had an ongoing program (under other sponsorship) in the area of low- and intermediate-temperature chemistry of hydrocarbons. This research, undertaken at atmospheric pressure, has potentially important applications to the chemistry occurring during knock. Drexel University will expand work on chemical studies in a static reactor to include gas sampling and analysis in a research engine on loan from Sandia National Laboratory. The objectives of this program are to develop an understanding of the oxidation chemistry of engine combustion processes and to determine fuel property effects on these processes. The scope of the research program is directed toward the study of hydrocarbon chemistry at low and intermediate temperature, with major emphasis placed on its relationship to autoignition and engine knock. Efforts are being concentrated on autoignition chemistry; the role and significance of the preignition end gas reactions and heat release in autoignition and knock; pressure effects of hydrocarbon oxidation mechanisms; and fuel chemistry effects on hydrocarbon decomposition processes. Experiments are being conducted using three separate, well-defined experimental systems; a static reactor, an atmospheric pressure flow reactor, and a knock research engine. These three complementary experimental systems are being used to examine chemical processes and fuel effects over a wide range of conditions important in engine combustion systems. Results from this project will provide a better understanding of the important chemistry and fuel-related problems in engine combustion systems.

Imperial College of Science and Technology
London, GB

86. *Experimental Measurements of Fuel Injection Processes*
Whitelaw, J.H.; Arcoumanis, C.

Imperial College will continue in situ measurements of time- and space-resolved velocity, turbulence, and concentration during fuel injection into a reentrant bowl configuration. Ensemble-averaged and instantaneous concentrations will be documented to illustrate the influence of injection characteristics, three-dimensionally, and rotational speed. These data will be compared with the results of the RPM two dimensional computer model that has been developed in parallel to simulate these processes.

Lawrence Livermore National Laboratory
University of California
Livermore, CA 94550
Physics Department

87. *Chemical Kinetics in Engines*
Westbrook, C.K.

Lawrence Livermore National Laboratory (LLNL) is responsible for developing and validating detailed and simplified global reaction kinetic mechanisms, to describe the ignition process, the rates of combustion, and the evolution of pollutant emissions. These kinetic mechanisms are incorporated into the developing computer models to predict performance, efficiency, and emission trends while engine design parameters are widely varied.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545
T Division

88. *Engine Combustion System Modeling*
Butler, T.D.

Ultraviolet and visible radiation from the sun and man-made sources affect living organisms in several different ways, some of which are harmful while others are beneficial. Modern technologies may alter the intensity and spectral distribution of solar radiation reaching the earth and thus alter the existing balance between the sun's harmful and beneficial effects. New man-made light sources also may alter this balance. Realistic evaluation of the possible biological hazards of visible and ultraviolet radiation requires an understanding of their various, sometimes antagonistic, effects. This project studies the damage inflicted on DNA irradiated in vitro and in vivo and relates specific types of molecular damage to cell death, mutation, and cancer induction. Focus is on developing procedures for quantitating the damage done to the DNA of human skin irradiated in situ and the subsequent repair of this damage.

Massachusetts Institute of Technology
Cambridge, MA 02139
Mechanical Engineering Department

89. *Fuels Chemistry and Emissions Interactions*
Keck, J.; Hochgreb, S.

This project will determine ignition delay times in the form of pressure-time profiles for fuel-oxidant mixtures after rapid compression. Fuels investigated include: gasoline blends, alkanes, aromatic hydrocarbons, ethers, alcohols, alkenes, and aldehydes. Insight gained from these studies will help define the characterization of

species and the chemical kinetic mechanisms describing their formation. The project will develop and test simple and accurate models of hydrocarbon oxidation that can be coupled with the 3-D fluid dynamic models to predict performance, fuel economy, and emissions.

Pennsylvania State University, University Park
University Park, PA 16802

90. *In-Cylinder Soot and NO Production*

Litzinger, T.A.

The objective of this program is to develop an improved understanding of the phenomenological nature of the in-cylinder processes of soot and NO formation and soot oxidation in direct-injection (DI) diesel engines. Measurements will be made in an optically accessible, single cylinder, DI diesel engine of the spatial and temporal evolution of soot and NO using planar imaging techniques. These measurements are intended to provide new insight regarding the interdependency of soot and NO emissions and lead to improved in-cylinder strategies for their control. To accomplish this objective, an experimental study will be performed using laser diagnostic techniques to observe soot and NO within the combustion chamber of a specially built DI diesel engine. Planar laser light scattering will be used to observe the soot, and laser-induced fluorescence will be used for the NO measurements. To couple the in-cylinder measurements of soot and NO to emissions, the particulate and NO_x exhaust emissions will also be measured. Engine parameters, such as injection timing and air temperature, will be varied to observe their effect on soot and NO. From this information, an in-cylinder approach to reducing both NO_x and particulate emissions may be formulated.

91. *Turbulent Flame Initiation*

Santavicca, D.A.

The project objective is to understand the effect of turbulence on ignition and early flame kernel growth under dilute charge conditions, both in terms of charge ignitability and the related problem in cyclic variability. Experiments will be conducted in a high-pressure turbulent flow reactor capable of simulating the pressure, temperature, equivalence ratio, and turbulence conditions that occur in an engine cylinder. The project will characterize both the turbulence intensity and the length scales, information critical to the development of turbulent combustion models. As part of this research, Pennsylvania State University will study the effect of incomplete fuel-air mixing on turbulent flame kernel growth; the effect of turbulent intensity and length scale on turbulent flame kernel growth; and the relative importance of thermal versus chemical effects on ignition flame kernel growth. Pennsylvania State University will also develop a spark-ignited, turbulent flame kernel growth model that incorporates the fractal turbulent flame kernel growth model.

Princeton University
Princeton, NJ 08544
Department of Mechanical and Aerospace Engineering

92. *DISC Engine Processes*

Bracco, F.

The project objective is to integrate the understanding of fuel injection processes and the fluid mechanics of combustion into the current multidimensional models. This integration involves the comparison of model predictions with the results obtained from well-defined experiments that isolate the controlling subprocesses. Focus is on developing and testing spray models. The models will eventually be incorporated into the KIVA multidimensional modeling code.

93. *Hydrocarbon Oxidation Chemistry*

Dryer, F.; Brezinsky, K.

Princeton University is developing chemical kinetic information to support and interpret emissions effects related to fuel characteristics for spark ignition engines, diesels and gas turbines. Present aspects of the work are relevant to improving how the blending characteristics of petroleum-derived fuels and fuel additives such as oxygenates affect hydrocarbon reactivity and emissions. This research involves the use of a variable-pressure flow reactor, to quantify the chemical kinetic processes under realistic conditions.

Sandia National Laboratories, Livermore
Livermore, CA 94551
Combustion Research Facility

94. *Diesel Engine Processes*

Dec, J.; Espey, C.; Carling, R.

This is a cooperative effort with Cummins Engine Company to contribute to the design of future diesel engines by developing an improved understanding of the critical in-cylinder combustion processes that lead to particulate and NO_x emissions. An optically accessible diesel engine will be used to measure where particulates are formed, location and timing of NO_x formation, fuel spray mixing, vaporization, and combustion rates. This data will be used to validate the 3-D computer simulation models developed.

95. *Two-Stroke Processes*

Green, R.; Carling, R.

This is a cooperative effort with General Motors to observe the flow field characteristics of the gas exchange process occurring during the scavenging of the exhaust products from an optically accessible two-stroke engine. Two methods of removal will be evaluated, crankcase and external blower scavenging. Optical methods will be used to provide GM with detailed knowledge on the gas exchange occurring, fuel injection and fuel-air mixture preparation, flame propagation, and the chemistry of combustion.

Southwest Research Institute
San Antonio, TX 78228-0510

96. Particulate Formation in Diesel Engine Combustion

Schwalb, J.; Ryan, T.W., III

This research uses a continuous flow simulator of a diesel combustion chamber to investigate the effect of turbulence length scales on the combustion process and the resultant emissions. The work will focus on determining the extent of the fuel spray jet and combustor wall interaction, the effect of fuel spray and wall impingement on geometry of the spray, primary jet breakup, and turbulence effects on emissions. The data generated by a well-defined system will be used to update the KIVA code in a cooperative effort with Los Alamos National Laboratory (LANL).

General Combustion Technology

Georgia Institute of Technology
Atlanta, GA 30332
School of Aerospace Engineering

97. Effect of Pulsations on Black Liquor Gasification

Zinn, B.T.; Jagoda, J.

This research investigates the use of pulse combustion to provide the energy required for the gasification of black liquor in fluidized beds. The work will determine to what extent the pulsations increase the heat transfer from the pipes to the bed material and within the bed, determine the effect of operating pressure on heat transfer within the bed, determine the optimum temperature of the process needed to gasify black liquor but prevent melting of the inorganic components, and determine the variability of the resultant synthetic fuel gas and the emissions produced from the combustion of the syn gas.

Lawrence Livermore National Laboratory
University of California
Livermore, CA 94550
Physics Department

98. Chemical Kinetics in Industrial Systems

Westbrook, C.K.

Lawrence Livermore National Laboratory (LLNL) is responsible for developing and validating detailed and simplified global reaction kinetic mechanisms to describe the formation of toxic species that are a byproduct from the combustion of refinery process fuel gas. These kinetic mechanisms are incorporated into developing computer simulation models to provide advanced burner designs for process heaters.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545
T Division

99. Spray Combustion System Modeling

Butler, T.D.

Los Alamos National Laboratory (LANL) is responsible for developing multidimensional computer models to simulate complex process occurring in continuous spray combustion systems. A 3-D computer model, KIVA-F90, is under development to analyze the coupled fuel spray, gas dynamics, combustion and pollutant formation reactions, and heat transfer applied to process heaters. The focus of the effort is on advancing efficient and effective means of computing an overall numeric solution that is graphically illustrated. This program is composed of detailed submodels that are being continuously updated and validated with experimental test results.

National Institute of Standards and Technology, Gaithersburg
Gaithersburg, MD 20899

100. Spray Diagnostics

Semerjian, H.G.

The objective of the National Institute of Standards and Technology (NIST) experimental program is to use a laboratory-scale spray combustion facility to investigate droplet evaporation, combustion, and particulate formation processes in spray flames, using both nonintrusive and intrusive techniques, and to delineate the effect of chemical and physical properties of the fuels. Research for this project includes droplet velocity distributions, polarization sizing techniques, and the effect of fuel properties. Emphasis will be placed on waste-derived liquid fuels containing aromatic hydrocarbons.

Sandia National Laboratories, Livermore
Livermore, CA 94551
Combustion Research Facility

101. Pulse Combustion Processes

Bramlette, T.T.; Keller, J.

This activity expands the successful pulse combustion project to scale up the Sandia Helmholtz combustor by a factor of 40:1 to validate the vortex dynamics computer code to model the multiphase, transient, highly-coupled, nonlinear flow field for burner design. This burner will involve temperature and fluid dynamic mixing control to achieve less than 7 ppm NO_x. This burner will also be used to validate the pulse combustor for the burning of liquid chlorinated compounds.

102. Internal Mix Atomizers

Edwards, C.

This research focuses on the understanding of how atomizer design impacts the structure of the flame and the resultant emissions. The work will study the atomization

and flame structure of heavy fuel oil flames using nonintrusive optical methods. Measurements will be made of the droplet atomization and dispersion of several atomizer designs.

103. Burner/Furnace Modeling

Edwards, C.

The development of the next generation computer codes will be based on large-eddy simulation (LES) models and take advantage of advances in massively parallel computer systems. The 2-D axisymmetric calculations using the turbulence model has proven to be inadequate to simulate the swirling gas-phase flow in furnaces. This work will develop a simulation where large-scale motion is explicit, and the small-scale turbulence is modeled.

THERMAL SCIENCES

Advanced Conversion Processes

Idaho National Engineering Laboratory
EG&G Idaho, Inc.
Idaho Falls, ID 83415

104. Advanced Two-Phase Flow Modeling: Eulerian–Lagrangian Model

Mortenson, G.

The objective of the generic two-phase flow and heat transfer model development is to provide a generalized tool of predicting heat transfer and pressure drop behavior for a wide spectrum of boiling–condensing two-phase flow operations in industrial equipment. In the Eulerian–Lagrangian modeling approach, the two continuous portions of the gas and liquid phases are represented as separate Eulerian fluids (bulk of the fluids are observed at fixed stations) in the same manner as existing two-fluid models, while the entrained droplets (in the continuous gas phase) and the bubbles (in the continuous liquid phase) are represented as discrete Lagrangian particles. In this way, flow regime transitions can be represented and predicted "mechanistically" as a consequence of more basic processes such as bubble and droplet coalescence, breakup, entrainment, and merging. Moreover, statistical effects from the distributions of droplet and bubble properties (size, velocity, and so forth) which are largely neglected in existing models, are automatically captured. Because it is not feasible to represent each droplet and bubble, groups of physically similar droplets and bubbles (obtained by random sampling) are used. The model and associated numerical solution procedure are initially being formulated in one space dimension. The extension to a corresponding 3-D model was initiated in FY 91 and will constitute the bulk of the effort in future years.

Jet Propulsion Laboratory
Pasadena, CA 91109

105. Alkali Metal Thermal-to-Electric Converter (AMTEC)

Fabris, G.

There are two objectives for the Alkali Metal Thermoelectric Converter (AMTEC) task: (1) to characterize and optimize the thermal performance of AMTEC cells utilizing large (full-tube) area electrodes and (2) to characterize the local temperature gradients within the cell that are important for fundamental understanding of device performance and may significantly affect stresses within the device. The recent focus of this task has been to conduct further experiments with large-area electrodes, including efficiency and thermal characterization, and to make the first measurements of the emissivities of both AMTEC electrodes and the beta-alumina solid electrolyte (BASE) surfaces. The task has also been successful in obtaining initial, somewhat crude, measurements of the emissivities of both electrode and BASE surfaces in an isothermal enclosure within a vacuum furnace. Both surfaces showed emissivities of 0.5 to 0.7, by comparison with standards also measured by pyrometry, and thermocouples within the enclosure. In addition, several tests were run in the electrode test cell (ETC) and the sodium vapor exposure test cell for periods of about 1000 hours; however, RTC test runs were not maintained longer than 200 hours.

106. Two-Phase Liquid-Metal Magnetohydrodynamic Generator

Fabris, G.

The primary objective of this project is to reduce the slip loss between gas bubbles and the liquid metal by the use of surfactants. Other potential improvements include (1) designing a mixer that creates a homogeneous laminar bubbly flow pattern instead of the turbulent slug-flow mixing observed in the past, (2) mixing at higher pressures (i.e., at lower void fractions where it is easier to achieve a bubbly flow pattern), (3) expanding the bubbly flow at a faster rate and under a much higher pressure ratio (about 20:1) without disturbing the flow and achieving a higher void fraction, (4) developing a more favorable dynamic-surface-tension distribution with enhanced heat transfer from the liquid to the gas (higher pressure ratio expansion) which will help to inhibit their coalescence, and (5) preventing additional coalescence of bubbles during expansion in the LMMHD generator as a result of surfactant-induced dynamic surface-tension effects. In FY 92, the construction of the major part of the liquid-metal blowdown loop that will be used to investigate effects of mixer and surfactants will continue.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

107. Thermoacoustic Engine Research

Swift, G.W.

A sound wave is usually thought of as consisting of pressure and displacement oscillations, but always attendant to pressure oscillations are temperature oscillations. The combination produces a rich variety of "thermoacoustic" effects, which can be harnessed to produce powerful, efficient heat engines such as prime movers, heat pumps, and refrigerators. The objectives of this research include (1) completing laboratory measurements confirming basic thermoacoustic energy-conversion theory; (2) developing improvements to the design code and documentation thereof, producing a code that can easily be used by other thermoacoustic research groups; and (3) developing experiments showing the tolerance of thermoacoustic effects to geometrical imperfections in heat-exchange elements. The principal focus is on a helium thermoacoustic engine because it is versatile and changes can be implemented inexpensively. Heat input and work output are being studied in detail. Based on current evidence, the work

output of the existing engine is in agreement with theory, but the heat flow is significantly higher than theory predicts. It is believed that the extra heat flow arises from unidentified hardware problems, not from any fundamental flaw in theory.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

108. Thermomagnetic Heat Pump Processes

Chen, F.C.

The objective of this project is to build a technology database based on an improved understanding of the fundamental thermophysical aspects of superconducting thermomagnetic energy conversion (TEC) processes. This knowledge will enable designers to develop environmentally safe and highly efficient TEC equipment for heating, refrigeration, and cryogen production as well as power generation. Specific goals will include (1) analyzing thermodynamic cycles and processes for TEC, (2) examining and simulating important cycle loss mechanisms, (3) conducting tests to delineate energy flow between thermal processes and working-media interactions, (4) identifying desirable working-medium thermophysical properties, and (5) investigating generic thermomechanical losses unique to regenerative and recuperative superconducting TEC concepts. Results in FY 91 showed that (1) the thermodynamic cycle irreversibility can be minimized by employing a regenerative cycle for the magnetic heat pump (MHP), (2) the MHP cycle performance varies strongly with the selected working media and the range of temperature lifts, and (3) the irreversibilities in a regenerator are one of the dominant losses in an MHP system. With a proper understanding of the regenerative-energy-transport process and the working-media and fluid interaction, the development of TEC systems can be successful.

109. Ammonia–Water Transport Properties

Chen, F.C.

The objective of this project is to systematically conduct single-tube tests to obtain transport properties of ammonia–water mixtures. The intention is to develop a sound engineering database covering a range of applications critical to the design, development, and scaleup of process equipment employed in advanced, binary working-fluid energy conversion industrial applications, such as Kalina power cycles and compression–absorption heat pumps. The initial focus of this project is on the condensing–absorbing process of ammonia–water mixtures on the outside of a single tube. The test conditions will be representative of ones corresponding to the Kalina power cycle, which is of interest to Exergy, Inc., under a fund-in Cooperative Research and Development Agreement (CRADA). The single-tube tests will include smooth, fluted, and Exergy supplied tubes. The tube orientations will include horizontal, vertical, and intermediate angles. The heat load, mixture concentrations, temperature range, and flow rate will also be varied so that extended transport characteristics of the mixtures can be obtained.

Pacific Northwest Laboratory
Richland, WA 99352

110. Bubble Dynamics

Liliegren, L.

The objective of this project is to provide data from which submodels describing the interaction between droplets, bubbles, and continuous liquid and gas phases may be obtained. Fundamental experimental investigations into bubble dynamics are being conducted to form and validate the constitutive relationships necessary for describing interfacial area transport and momentum transfer in bubble swarms and the motions of bubble pairs. The first set of experiments are primarily oriented towards developing the interfacial area transport equations required by Pacific Northwest Laboratory's (PNL's) four-field model, but also providing useful data for validation of Idaho National Engineering Laboratory's (INEL's) Eulerian–Lagrangian code. Initial experimental investigations currently focus on the phenomena of bubble coalescence, bubble shape, and drag. Additional investigations on bubble interfacial area growth–reduction mechanisms are required to develop constitutive relationships for all phenomena described in both the INEL and PNL numerical models.

111. Advanced Two-Phase Flow Modeling: Four-Field Model

Lombardo, N.

The objective of the generic two-phase flow and heat transfer model development is to provide a generalized tool of predicting heat transfer and pressure drop behavior for a wide spectrum of boiling–condensing two-phase flow operations in industrial equipment. The four-field modeling approach treats the continuous liquid, continuous vapor, bubbles, and droplets as four distinct fields in the flow. The fields interact both thermodynamically (evaporation and condensation) and mechanically (entrainment, deentrainment, coalescence, breakup, and drag) across their interfaces. The essential feature is the application of the interfacial area transport concept to handle the variation in dimensions of the discrete fields. Extension of the four-field model to higher void fractions could potentially eliminate the need for flow-regime maps, and the abrupt transitions predicted for flow behavior that are inherent to models using flow-regime maps. The extension of the four-field model to multicomponent mixtures, while challenging, is a relatively straightforward evolution of the multifield modeling capability, if multicomponent values of the thermodynamic and transport properties can be defined. With the synergistic linking with the Molecular Dynamics Modeling of Multicomponent Mixtures project, one has the potential for developing "working fluids by design".

112. Molecular Dynamic Modeling

Palmer, B.

The purpose of this program is to develop computational methods involving molecular dynamics (MD) and Monte Carlo (MC) modeling techniques to calculate thermodynamic and transport properties of engineering interest for both single and multicomponent fluids. During FY 91, effort on developing a methodology for calculating the absolute evaporation rate of a simple liquid using molecular-dynamics simulations was completed. This is a

prototype problem for transport across the liquid–gas interface. Transition-state theory (TST) is being used to calculate a preliminary value of the rate, using free-energy differences and accounting for the effect of surface interactions on molecular motions. Models are also being developed for doing realistic simulations of a prototype binary mixture under constant pressure–constant temperature conditions. Water–carbon dioxide mixtures have been chosen for initial investigations.

Heat and Mass Transfer Research

Argonne National Laboratory
Argonne, IL 60439

113. Fouling Mechanisms

Panchal, C.B.

The objective of the fouling research program is to understand the mechanisms of the fouling process so that equipment may be designed to minimize the fouling buildup and to mitigate the fouling after it forms. An important part of the fouling research is to determine the interactive effects of fouling and enhancement mechanisms in order to optimize the enhancement geometry for maximizing the thermal performance with minimum propensity for fouling. Efforts have been focused in two areas: (1) fouling and enhancement interactions and (2) organic fluid fouling. Investigations of the interactive effects of fouling and heat-transfer enhancement mechanisms have yielded the first long-term fouling rate comparison of plain and enhanced tubes. While the commercial enhanced tubes foul at a faster rate, the overall thermal performance was improved over the plain tubes based on two years of operation without cleaning. Organic-fluid fouling has focused on the development of an analytical method of determining the rate controlling mechanisms and effects of the physical parameters. The analytical method will be used to determine the threshold conditions of fouling. An experimental program is currently being conducted to obtain data for validating the analytical fouling model. Two major tasks have been completed in this area: (1) a critical review of literature and (2) the formulation of an analytical fouling model.

114. Direct-Contact Analysis

Panchal, C.B.

The objective of this research is twofold: (1) to extend the existing Argonne National Laboratory (ANL) model to include mass transfer effects for drying applications and (2) to develop a basic understanding of the interfacial heat and mass transfer encountered in separation processes. Although direct-contact processes are generally related to the separation technologies, the scope of the research element was expanded to include the mass-transfer aspects. In the present structure of the research approach, it includes absorption, adsorption, drying, and membrane separation applications. This research element also includes heat- and mass-transfer processes in the advanced energy conversion systems (e.g., Kalina cycle and chemical heat pumps).

115. Heat Transfer Surface Enhancements

Rabas, T.J.

The objective of this research is to improve energy efficiency in existing energy-conversion and process plants by optimizing the performance of existing types of heat exchangers. One major thrust is to advance the knowledge gained, which will be incorporated into a database made available to designers of state-of-the-art heat exchangers. Major progress and accomplishments in FY 92 are (1) a numerical analysis effort to determine the effects of the disruption shape and Prandtl number; (2) the use of the transient, liquid-crystal method to obtain local heat-transfer coefficients for square and circular enhanced passages; (3) mean heat-transfer and pressure-drop results for 24 enhanced tubes with air (Pr = 0.7) as the test fluid; and (4) the extension of a single-phase enhancement data bank.

116. Phase Change Heat Transfer

Wambsganss, M.W.

This research is comprised of two types of projects: (1) projects directed toward generic two-phase flow and heat-transfer model development, supported by experimental studies to determine the correct constitutive relationships and (2) projects focused on the two-phase flow in particular configurations for which existing knowledge is inadequate to provide design guidance. Two-phase dynamics (flow patterns and pressure drops) and flow boiling in small channels typically representing plate-fin heat exchanger geometries are currently under investigation. In FY 92, the research was focused on the flow-boiling experiments and on the documentation of results from adiabatic, two-phase flow experiments with air–water mixtures in small, rectangular channels (4.04 x 1.70 mm). Single-phase and flow-boiling heat-transfer experiments with R-113 in a small (2.92 mm) diameter tube were performed for the purpose of validating the instrumentation, data-acquisition and processing system, and analysis methods, and to provide reference data against which the subsequent rectangular channel data can be compared. Current efforts focus on performing heat-transfer experiments utilizing this channel.

MATERIALS

Engineered Industrial Materials

Georgia Institute of Technology
Atlanta, GA 30332
Department of Materials Engineering

117. Thin-Wall Hollow Ceramic Spheres from Slurries

Cochran, J.K.

The goal of this project is to develop processes for economically fabricating hollow, thin-wall spheres from conventional ceramic powders using dispersions and to assess their potential use. The feasibility of producing monosize hollow spheres of many ceramic compositions on a production basis has been successfully demonstrated. The properties of the spheres (i.e., mechanical strength and thermal conductivity) have been documented and mathematical modeling of the sphere-forming process has been successful. Current research has three areas of emphasis: (1) to reduce thermal conductivity at high temperatures using IR opacifiers in the sphere walls, (2) to convert the liquid slurries used to form spheres from the present organic-based to an aqueous-based system, and (3) to disseminate information about sphere technology and properties to U.S. industry.

Lawrence Livermore National Laboratory
University of California
Livermore, CA 94550
Department of Chemistry and Materials Science

118. Three-Dimensional X-Ray Tomography of Crack-Resistant Composites

Kinney, J.H.; Saroyan, R.A.

X-ray tomographic microscopy (XTM) is a new technique for noninvasively imaging materials' microstructures in three dimensions. The microporosity between individual filaments in the fiber bundles, the channel porosity between individual cloth layers, and the connectivity of the large through-ply holes that remain after processing can all be examined without destroying the sample. Current XTM research is focused on monitoring the chemical vapor infiltration (CVI) processing of silicon carbide matrix–Nicalon fiber composites. Direct visualization of the evolving microstructure during CVI will be compared to model calculations and correlations between processing conditions such as temperature and pressure on density and mechanical properties.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

119. Synthesis and Design of Intermetallic Materials

LeSar, R.A.; Petrovic, J.J.; Rollett, A.D.

The purpose of this project is to develop and design intermetallic materials using the composite approach to obtain fracture resistance in brittle matrices. Efforts are focused on a high-temperature structural material, $MoSi_2$, because of its good oxidation resistance and ductility at elevated temperatures. Micromechanical modeling of the complex microstructure of these composites has been successful in showing which toughening mechanisms are significant. The modeling has also demonstrated that the dispersion of the toughening additions in the silicide matrix is critical to maximizing the toughening effect.

Oak Ridge National Laboratory
Oak Ridge, TN 37831
Metals and Ceramics Division

120. Ni_3Al Technology Transfer: Castability and Weldability of Ni_3Al

Alexander, D.J.; Santella, M.L.; Sikka, V.K.

Ductile Ni_3Al and Ni_3Al-based alloys have been identified for a range of applications. These applications require the use of materials in a variety of product forms such as sheet, plate, bar, tubing, piping, wire, and castings. Although significant progress has been made in the melting, casting, and near net shaping of nickel aluminides, some important technological issues related to the processing, fabrication, and mechanical behavior of these alloys remain unsolved. The objective of this project is to facilitate the transfer of intermetallic alloy technology to industry by resolving technical issues constraining the industrial application of alloy systems and by providing a forum for exchange of data by industrial suppliers and users. This includes castability (fluidity, hot shortness, and porosity), weld repairability of castings, hot workability of cast ingots, and fracture toughness properties.

121. Metallic and Intermetallic Bonded Ceramic Composites

Alexander, K.B.; Becher, P.F.; Liu, C.T.; Schneibel, J.H.; Tiegs, T.N.

To improve the reliability of ceramic components, new approaches to increasing the fracture toughness of ceramics are required. The objective of this project is to establish a framework for the development and fabrication of metallic and intermetallic-reinforced ceramic matrix composites with improved fracture toughness and fatigue resistance. The incorporation of metallic phases into a ceramic matrix allows for local plastic deformation. This deformation acts to dissipate the strain energy introduced by an applied

stress, thus increasing the fracture toughness of the composite. The research will focus on the development of alumina-based as well as nonoxide-based (AlN, TiN, TiC, and WC) ceramic composites reinforced with ductile nickel aluminide alloys. This work will also identify relationships between material properties, structure, and processing. Reinforced ceramic matrix composites have potential use in advanced industrial applications.

122. Advanced Ordered Intermetallic Alloy Development

George, E.P.; Horton, J.A.; Liu, C.T.

The objective of this project is to develop low-density, high-strength intermetallic alloys for structural use in advanced heat engines and energy conversion systems. Many ordered intermetallics have attractive high-temperature properties such as excellent oxidation and corrosion resistance, high-elevated-temperature strength, low material density, and excellent shape-memory effects. However, brittle fracture and poor ductility limit their use as engineering materials. The general approach is to improve the ductility and fabricability of ordered intermetallics by controlling the crystal structure. Current efforts are focused on the development of a new generation of materials including (1) NiAl alloys with high-temperature capability, (2) TiAl and $TiAl_3$ alloys with high specific strength, and (3) shape-memory alloys based on NiAl–Ni_2Al.

123. Development of Weldable, Corrosion-Resistant Iron–Aluminide Alloys

Goodwin, G.M.; Maziasz, P.J.

The objectives of the project are (1) to develop weld-overlay FeAl and other intermetallic alloys as coatings and claddings on intermetallic and conventional structural materials and (2) to develop weldable and corrosion-resistant FeAl alloys. Efforts on FeAl development have shown that environmental effects (hydrogen embrittlement) generally are the mechanisms limiting room-temperature ductility, and that proper control of alloy composition, microstructure, and surface condition (oxide layer) significantly improves ductility. Current efforts are focused on the development of FeAl materials for coatings including weld-overlay coatings and claddings. Studies have shown that such coatings are feasible, but that hydrogen-related cold-cracking of the weld-deposited FeAl and the dilution zone that forms between overlay deposit and the base material are issues that still need to be addressed.

124. Materials by Design: New Ordered Intermetallic Alloys

Hazzledine, P.M.; Nicholson, D.M.

The purpose of this work is to develop and use theoretical tools useful for the design of ductile high-temperature intermetallics. This objective will be reached by the use of dislocation theory, the embedded atom method, simulation, and first principles local density calculations. The program will strive to determine alloy additions that ductilize intermetallics. Applications of this technology include calculating the electrical conductivity in the commercial alloy Hastelloy-B, which explains the peculiar drop in resistivity after cold working, and calculating the ordering energy of NiAl. With further research, these studies may explain why the maximum ductility occurs at stoichiometry and is improved by very small amounts of ternary addition.

125. High-Temperature Precipitation-Strengthened Iron Aluminides and Other Intermetallic Alloys

Hubbard, C.R.; Maziasz, P.J.; Sikka, V.K.

The purpose of this project is to produce precipitate- and microstructure-based strengthening of the high-temperature B2 phase Fe_3Al type alloys, while maintaining the best possible combinations of weldability, room-temperature ductility, and other enabling properties. This project will explore the effects of solute additions aimed at producing fine, stable dispersions of carbides or other precipitate phases to strengthen the B2 phase at high temperatures. Results reveal that modified alloys have improved room-temperature ductility and creep-rupture strength relative to the as-fabricated material. Correlation of this data with high-temperature X-ray diffraction data on the transition temperature and kinetics suggest that retaining the B2 phase is important to obtaining room-and high-temperature properties behavior.

126. Polymers with Improved Surface Properties

Lee, E.H.; Lee, Y.; Mansur, L.K.

The purpose of this project is to enhance and improve the durability, dielectric–electric–magnetic–IR properties of polymers using surface modification treatments, and to correlate changes in microstructure and microcomposition with surface property changes. Research will emphasize (1) modification of surface-sensitive properties of polymers by multiple-ion beam treatments; (2) characterization of induced changes in microstructure, microcomposition, and properties by means of analytical electron microscopy, ion scattering–nuclear reaction techniques and mechanical testing; and (3) relation of ion beam processing parameters to microstructure and properties in order to develop principles for improved materials. Results indicate that near-surface hardness values can be significantly improved for shallow implants compared to unimplanted polymers and that shallow implants can be used to improve surface mechanical properties of polymers.

127. Development of Corrosion-Resistant Iron–Aluminide Alloys

Liu, C.T.; David, S.A.

The objective of this project is to identify an FeAl composition with the best combination of room temperature ductility and corrosion resistance in oxidizing molten nitrate salt environments. A binary base composition of FeAl was selected on the basis of tensile strength results, creep strength, fabricability, and corrosion resistance. Minor alloying additions increased the room temperature tensile ductility by fivefold compared to the pure binary aluminide. FeAl compositions with excellent corrosion resistance in molten nitrate salts were also identified. Weldability has also been found to be a strong function of composition and welding parameters. Crack-free welds have been obtained in FeAl alloys with controlled minor alloy additions. Future activities include (1) alloy design

to improve creep strength, while maintaining ductility; (2) evaluation to determine resistance of FeAl compositions to high-temperature oxidation; (3) scale up to industrial size heats and further interactions with industry.

Sandia National Laboratories, Albuquerque
Albuquerque, NM 98195

128. Composites through Reactive Metal Infiltration

Loehman, R.E.; Ewsuk, K.G.

Metal matrix ceramic composites have been fabricated using a novel reactive metal infiltration processing technique. The process involves reacting a molten metal with a ceramic preform to produce a fine scale composite microstructure of ceramic particles within a continuous metal matrix. Experimental variables include the reactive metal and ceramic compositions, and the processing temperature and atmosphere. Advantages of reactive metal infiltrated composites include lower temperature and near net shape processing of ceramic composites and improved toughness compared to traditional ceramics. Current efforts are focused on characterizing the aluminum–mullite system.

Idaho National Engineering Laboratory
EG&G Idaho, Inc.
Idaho Falls, ID 83415
Materials Technology Division

130. Superior Metallic Alloys through Rapid Solidification Processing by Design

Flinn, J.E.

The industrial sector requires metallic alloys whose properties, performance, and reliability extend beyond those obtained from current processing practices. These needs can be fulfilled by metallic alloys that have fine and stable (to high temperatures) microstructure. Rapid solidification processing (RSP) during powder atomization and control of the minor elements, such as oxygen and strong oxide formers, can produce metallic alloys with superior properties and performance compared to conventionally processed alloys. Efforts will continue to collaborate with U.S. industries in applying rapid solidification processing in combination with composition adjustments to produce superior metallic alloys.

Materials Manufacturing Technologies

Idaho National Engineering Laboratory
Idaho Falls, ID 83415

129. Magnetic Field Processing of Inorganic Polymers

Kunerth, D.C.; Peterson, E.S.

The application of magnetic fields during processing has been shown to modify the physical and chemical properties of inorganic polymers. Development of this technology will significantly improve current materials as well as lead to new materials for other applications. The objective of this project is to investigate and demonstrate the use of magnetic field processing, to modify the properties of inorganic-based polymers, and to develop the basic technical knowledge required for industrial implementation. Current results have shown that (1) the physical and chemical properties of polyphosphazene polymers have been modified using magnetic field processing, (2) the membrane morphologies and transport properties can be changed with the application of magnetic fields, and (3) the polymer can be textured on the molecular level.

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720
Applied Science Division

131. Development of Improved Aerogel Superinsulation

Hunt, A.J.

The purpose of this project is to develop methods of producing new aerogel-based materials using sol–gel processing and supercritical solvent extraction. Aerogel is a porous, low-density, nanostructured solid with many unique properties including transparency, very high thermal resistance, and low sound velocity. The primary challenge is to develop new processing methods to prepare aerogel with improved properties for a cost effective, high-performance thermal insulation. For example, aerogel can be substantially improved by adding nanostructured phases to increase the thermal resistance by reducing radiative heat transfer inside the material. Aerogel processing techniques may also be used to make other nanocomposite materials, including new magnetic materials. Applications for aerogel-based materials, include multicomponent ceramics, catalyst substrates, transparent porous solids, and high-performance thermal insulators that may replace existing chlorofluorocarbon (CFC)-containing foams currently used in refrigerators, water heaters, and industrial plants.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

132. *Microwave-Assisted Chemical Vapor Infiltration*

Currier, R.P.; Devlin, D.J.

The purpose of this investigation is to develop a viable microwave-assisted process for the rapid production of ceramic matrix composites of arbitrary geometry by chemical vapor infiltration (CVI). The potential advantage in using microwaves is to heat the substrate internally, giving rise to "inverted" thermal gradients. With the internal region of the substrate hot, cool reactant gases penetrate inward prior to the onset of reaction. Consequently, deposition occurs from the inside out. This could offer several advantages over conventional technologies including (1) removing constraints on substrate geometry; (2) obtaining more spatially uniform, high density composites; (3) shortening processing times; and (4) machining to reopen closed pores should not be necessary since densification would occur from inside out.

133. *Polymerization and Processing of Organic Polymers in a Magnetic Field*

Elliott, N.E.; Jahn, R.K.; Liepins, R.

The purpose of this project is to evaluate and model the effects of magnetic fields on polymers during polymerization, solidification, and processing in order to improve, modify, and control the mechanical, physical, optical, and electrical properties. The orientation of polymers in a magnetic field and subsequent polymerization can improve the various properties of the material. Current research has shown that magnetic field processing of epoxy resins had a significant positive effect on tensile strength, tensile modulus, reduced water absorption, increased hardness, and improved adhesion properties. The work at Los Alamos National Laboratory (LANL) emphasizes the polymerization and processing of liquid-crystalline polymers, nonliquid-crystalline polymers, and organic composites (epoxy prepregs). Quantitative correlations have been made between the properties and structure of the material prepared with and without the presence of a magnetic field. Research will continue to focus on dynamic "in-process" magnetic field processing of a liquid-crystalline polymer film.

134. *Microwave-Driven Spray Drying of Ceramic Powders*

Gac, F.D.; Katz, J.D.; Vogt, G.J.

The purpose of this project is to develop generic microwave processes by the direct coupling of microwave power for the spray-dry preparation of homogeneous oxide powders from aqueous and organic aerosols and for the drying and calcining of green filaments to produce ceramic fibers. Microwave-driven spray drying and filament processing are energy-efficient alternatives to the conventional thermal processing of aerosols and filaments. In thermal processing, thermal energy is transported from a hot gas or hot solid surface through the exterior surface toward the center of the aerosols and filaments. In microwave-driven processing, microwave energy is directly coupled to the entire body of aerosol particle and filament by volumetric absorption of the electric field. The advantages of microwave processing are the direct rapid heating by the volumetric coupling of clean energy without chemical contaminants from fuel gas heating and from hot reactor surfaces, shorter processing time, and the potential of novel microstructures due to rapid heatup as the filament is drawn through the microwave cavity.

135. *Conducting Polymers: Synthesis and Industrial Applications*

Gottesfeld, S.; Redondo, A.

This project is pursuing new methods for the synthesis of electronically conducting polymers, and the development of new industrial applications for these materials that will result in significant reductions in energy usage or industrial waste. Applications addressed include (1) improved industrial metallization methods that could replace current costly and environmentally damaging technologies, (2) supercapacitors that could save large amounts of energy when introduced in power trains of electric vehicles, (3) corrosion resistant conductive coatings, and (4) electrochromic conducting polymer films for variable opacity windows.

Materials Science and Technology Division

136. *Microwave Joining of SiC*

Blake, R.D.; Katz, J.D.

The purpose of this work is to develop and optimize a joining method that can be applied to large-scale fabrication of components such as radiant burner tubes and high-temperature, high-pressure heat exchangers. Efforts were focused on optimizing the properties of SiC–SiC joints made using microwave energy and this resulted in a 3-μm thin silicon interlayer. In addition, research on reaction-bonded silicon carbide, which contains residual free silicon, showed no interlayer. Current efforts are focused on forming a carbide interlayer through an in situ reaction.

Michigan Biotechnology Institute
Lansing, MI 48909

137. *Amylose-Styrene Maleic Anhydride Copolymer Composites*

Argyopoulos, D.; Nie, L.; Narayan, R.

The high demand for use of renewable sources has increased the interest of employing natural polymers (lignocellulosic, starch) in the chemical industry. One potential application is as fillers or reinforcements in a synthetic polymer matrix. The fine-particle size and narrow-particle size distribution of some starches, together with the low price and density compared to other spherical fillers (like glass spheres) are a few advantages of starch fillers. The purpose of this project is to develop and test the properties of various styrene maleic anhydride copolymers reinforced with a high-amylose starch filler.

138. Engineering of Polypropylene-Lignocellulosic Composites by Reactive Extrusion

Mohanakrishman, C.K.; Narayan, R.

The purpose of this project is to evaluate lignocellulosic materials as blend components in the preparation of thermoplastic matrices. One of the main concerns in any polymer blend system is the interfacial adhesion between the components of the blend. Blends of lignocellulosics with synthetic polymers exhibit high-interfacial tension and low adhesion, resulting in materials with poor mechanical properties. Chemical functionalities, specifically the anhydrides, have been used as adhesion promoters in polymer systems. In this research, an effort has been made to react the anhydride functionality with the components of the blend system, instead of simply mixing it in as an additive. Polymer modification using reactive extrusion produced maleic anhydride functionalities in a copolymer that were subsequently employed in the generation of in situ grafts between the copolymer and the lignocellulosic component. Blends of this maleated polymer with the lignocellulosic material exhibited improved tensile strength and tensile modulus.

National Renewable Energy Laboratory
Golden, CO 80401
Chemical Technologies Research Branch

139. Chemical Recycling of Plastics

Chum, H.L.; Czernik, S.; Evans, R.J.; Tatsumoto, K.

This research activity is aimed at developing cost-effective and environmentally benign processes for recovering mixed plastics from various sources, such as auto-shredder waste, carpet waste, and other source-separated mixed plastic streams. Current efforts are directed at the identification of experimental conditions for the chemical recovery of monomers and other high-value chemicals from plastic mixtures using controlled catalytic and thermal processes. The National Renewable Energy Laboratory's (NREL's) molecular-beam mass spectrometer is being used to detect real-time products of these processes and establish conditions for industrial development. Chemical recycling technology has been applied to the recovery of caprolactam from waste nylon carpet and to the recovery of dimethylterephthalate from positron emission tomography (PET) in mixed-waste plastic bottles.

Oak Ridge National Laboratory
Oak Ridge, TN 37831
Metals and Ceramics Division

140. Microwave Sintering of Composites

Beatty, R.L.; Becher, P.F.; Janney, M.A.; Kiggins, J.O.; Kimrey, H.D.

The purpose of this project is to develop ceramics for energy conversion systems with improved strength, toughness, reliability, and uniformity of properties using microwave processing to engineer and control critical component microstructures. The approach combines both experimental process development and modeling to provide an understanding of microwave processing that can be used in industrial applications. Current efforts focus on (1) developing zirconia-toughened alumina, (2) measuring the mechanical properties of zirconia-toughened alumina, (3) testing the dielectric properties, (4) characterizing the thermophysical properties of ceramics, and (5) modeling the heating of an insulated ceramic body in a single-mode microwave cavity.

141. Chemical Vapor Infiltration of Ceramic Composites

Besmann, T.M.

This project is designed to develop continuous fiber reinforced TiB_2 and SiC matrix materials. TiB_2 materials may be useful as Hall–Heroult aluminum smelting cathodes having substantially improved properties. Carbon cathodes currently require significant anode-to-cathode spacing in order to prevent shorting, causing significant electrical inefficiencies. The TiB_2 composite is fabricated through chemical vapor infiltration, producing a high-purity TiB_2 matrix without damaging the relatively fragile plain-weave carbon fibers. Current efforts have focused on producing uniform composite specimens at the elevated temperatures required to prevent detrimental chlorine retention. Resulting samples exhibited chemical stability in short exposures (24–48 hours) to molten aluminum. Efforts will continue to design and evaluate potential fiber reinforcements, fabricate test specimens, and test the materials in a static bath and lab-scale Hall cell.

142. Advanced Microwave Processing Concepts

Lauf, R.J.

The purpose of this project is (1) to explore new techniques and uses for microwave processing, including multilayer ceramic capacitors and polymer-matrix composites and (2) to develop variable-frequency microwave sources since existing microwave sources are confined to extremely narrow frequency ranges. The new variable microwave process will permit (1) more efficient use of microwave energy in processing of materials by being able to operate at optimum frequency or change the frequency as the material is heated and (2) more effective microwave field uniformity that allows for the uniform heating of single and multiple parts in furnaces. Current efforts are focused on the sintering of multilayer capacitors. Multilayer capacitors will provide an opportunity to study the effect of internal metallic phases on the behavior of parts during microwave processing.

Pacific Northwest Laboratory
Richland, WA 99352

143. Biomimetic Thin-Film Synthesis

McVay, G.L.; Rieke, P.C.; Tarasevich, B.J.

The objectives of this project are (1) to develop a method of forming artificial organic interfaces onto polymer and oxide substrates and (2) to demonstrate biomimetic thin-film deposition of various materials. Organic molecules can be attached to substrates and used to promote deposition of materials from solution. This is a similar approach used

by biological organisms in the formation of structural materials such as shells, bones, and teeth. The goal of this project is to tailor the organic interface to have various surface end-group sites densities, site functionalities, and site structures in order to control the properties of the inorganic deposit such as orientation, phase, and deposition location. Protective coatings for corrosion-, chemical-, and abrasion-resistant applications are currently under investigation in cooperation with the automotive industry. In addition, oriented, anisotropic, magnetic iron-oxide films are being developed for use as magnetic storage devices.

Polytechnic University
Brooklyn, NY 11201

144. Recoverable Thermosets

Tesoro, G.C.; Wu, Y.

The principal objective of this project is to develop viable approaches to the recovery of materials of value from cured unsaturated polyester resin for the purpose of providing new avenues to industry participation and potential technology transfer efforts. Current research efforts focus on investigating the chemical reactions of cured unsaturated polyester yielding well-characterized products, and identifying potential applications of compounds recovered. Neutral hydrolysis of cured unsaturated polyester resins was shown to be a viable approach to the solubilization of the thermosets and to the recovery of chemical compounds in good yields. In addition, potential applications of the recovered products have been explored with promising results.

Sandia National Laboratories, Albuquerque
Albuquerque, NM 98195
Inorganic Materials Chemistry Division

145. Chemically Specific Coatings

Doughty, D.H.; Frye, A.C.

Chemically selective films have potential application in membrane, chromatographic separation and chemical sensor technologies. While many techniques exist to prepare chemically specific coatings, sol–gel processing offers substantial advantages in being able to tailor physical and chemical properties of the coatings. Pore size, pore size distribution, pore volume, surface chemistry, and composition can be varied to provide optimal selectivity. Moreover, surface derivitizing reagents have been used to modify surface chemistry. The goal of this project is to develop a new class of chemical sensors through sol–gel processing that can be used to process monitors to improve process energy efficiency. Films have been applied to quartz oscillators in order to study the selectivity of their interactions with aqueous solutions. In addition, inorganic polymeric films have been applied to porous ceramic supports with the goal of preparing sol–gel metal-oxide films for gas separation.

Sandia National Laboratories, Livermore
Livermore, CA 94550

146. High Deposition Rate Chemical Vapor Deposition

Allendorf, M.D.

Comprehensive models, including detailed gas-phase and surface chemistry coupled with reactor fluid mechanics, are required to optimize and scale up chemical vapor deposition (CVD) processes. Several investigators have proposed models that simulate aspects of silicon carbide (SiC) CVD processes; however, these models predict only deposition rates and not deposit composition. Therefore, the purpose of this investigation is to develop a quantitative understanding of the chemical and physical mechanisms that result in high-deposition rates and fully dense materials from innovative high-temperature ceramic synthesis processes. Current results indicate that gas-phase chemistry is an important element in determining both the deposition rate and the elemental composition. Research will continue with attempts to model the gas-phase chemistry occurring during SiC CVD.

University of Southern Mississippi
Hattiesburg, MS 39406
Department of Material Science

147. Improvement of Wood Properties by Impregnation with Multifunctional Monomers

Mathias, L.J.

The objective of this project is to develop new, commercially applicable methods of fabricating wood–polymer composites (WPC) with improved dimensional and degradation stability, and improved physical properties. The approach is based on a new monomer, ethyl α-hydroxymethylacrylate (EHMA), that has alcohol and ester groups capable of penetrating in interacting with the wood components. Initial results have provided (1) a reliable laboratory scale synthesis of the new monomer EHMA from inexpensive acrylates and formaldehyde; (2) a WPC with excellent stability and improved physical properties; and (3) an extensive database for southern pine and balsa wood.

Thermo Electron Technologies Corporation
Waltham, MA 02254

148. Development of Chemical Vapor Composite Materials

Reagan, P.

The purpose of this project is to develop a reliable, flexible, and economic process to fabricate strong, fracture-tough ceramic composites to net shape in one step without machining. The chemical vapor composites (CVC) process has the potential to reduce the high costs and the multiple fabrication steps presently required to produce ceramic composites. Composites are fabricated by simply mixing powders and/or fibers with vapor reactants that are transported and codeposited on a hot machined

substrate. Current efforts are focused on the development of the CVC process with various powder and fiber combinations in a silicon carbide matrix.

University of Wisconsin at Madison
Madison, WI 53706
Department of Forestry

149. Plastic Wood

Young, R.A.; Rowell, R.M.

The purpose of this work is to develop a lignocellulosic-based composite from combinations of lignocellulosic and synthetic materials. Wood-based fiber and plastics can be used to produce a wide spectrum of products ranging from large market commodity products where performance requirements are minimal, to low-volume but high-value-added specialty products with rigorous performance requirements. Fiber technology, fiber modification, and bonding performance can be used to manufacture wood–plastic composites with uniform densities, durability in adverse environments and high strength. Current efforts in this project have been focused on developing a technique to estimate the shear strength in wood–thermoplastic systems, in order to optimize strength properties of cellulosic–thermoplastic composites.

CATALYSIS/BIOCATALYSIS

Bioprocess Engineering

Allied Signal, Inc.
Des Plaines, IL 60017
Engineered Materials Research Center

150. Reactions Catalyzed by Immobilized Enzymes in Organic Solvents

Zemel, H.

To extend the practical use of enzymes to industrially feasible processes, the use of immobilized enzymes in organic media will be studied for typical condensation reactions (i.e., lipase-catalyzed synthesis of esters like chiral precursors of phenoxyacetic-acid-derived herbicides). Already, lipases have been shown to catalyze transesterification reactions in organic solvents. The generic physicochemical principles on which this technique relies will be studied in detail: the role of the support geometry and surface, the influence of water activity in the organic phase, the influence of pH memory, and the effect of coimmobilized enzyme activators. This approach toward a more detailed understanding of immobilized enzyme reactions will lead to a wider range of enzyme applications in organic syntheses.

Massachusetts Institute of Technology
Cambridge, MA 02139

151. Enzymes for Use in Organic Solvents

Klibanov, A.M.

A major obstacle in using enzymes as practical catalysts in organic chemistry is the necessity to conduct enzymatic reactions in water, which is a poor medium for most industrial chemical processes. For example, the enzyme polyphenol oxidase in principle has a great potential for selective hydroxylation of aromatic compounds, an often desirable but very difficult problem in organic chemistry. However, polyphenol-oxidase-catalyzed oxidations cannot be conducted in water on a preparative scale because (1) most phenolic substrates are only slightly soluble in water; (2) quinones, formed as the product of the enzymatic oxidation, spontaneously polymerize in water; and (3) during that polymerization the enzyme is chemically modified and consequently inactivated. A novel approach is being implemented where an enzyme is lyophilized from an aqueous solution containing an appropriate ligand, then washed with an organic solvent to remove the ligand. Preliminary results indicate that the enzyme, while dry or in organic solvents, retains the conformation induced by the ligand and has enhanced catalytic activity, altered specificity, and greater stability. This phenomenon will be investigated to determine its scope and generality, with the objective of developing a rationale for alteration of enzyme characteristics as desired (e.g., to increase and retain activity or change specificity).

Oak Ridge National Laboratory
Oak Ridge, TN 37831
Chemical Technology Division

152. Immobilized Cell Bioreactor and Multi-Phase Immobilized Bioreactor

Scott, C.D.

Development of the Oak Ridge National Laboratory (ORNL) immobilized cell bioreactor for the production of ethanol from corn and sugar byproducts by *Saccharomyces* and *Zymomonas* has increased the bioreactor productivity by more than an order of magnitude and the yield of ethanol to about 98% of theoretical. It is a tubular continuous flow fluidized-bed bioreactor with the biocatalyst trapped in beads that remain in the bioreactor while the substrate solution flows through it. The project is cofunded by the National Corn Growers Association, St. Louis, Missouri. The use of dense product-absorbing beads in the continuous flow reactor has already been shown to meet the necessary physical requirements, namely that they can be added at the top of the column and pass slowly through the bioreactor for collection at the bottom of the column. They can thus be separated from less dense cell-containing beads that are retained within the fluidized bed of the bioreactor. In the case of lactic acid fermentation, it has been shown that the lactic acid can be continuously removed, better pH control can be attained, and that the product can be removed from the beads and the beads regenerated for reuse. Research is now focused on engineering scaleup of the advanced bioreactor design.

Tufts University
Medford, MA 02155
Department of Chemical Engineering

153. Electrochemical Oxidations and Reductions in Fused Salts

Stoukides, M.

High-temperature proton and oxygen ion conductors can be applied in heterogeneous catalysis to electrochemically modify the catalytic rates of hydrogenation and oxidation reactions. In this project, the electrocatalytic methane upgrading to dimerized products and to synthesis gas is under investigation. Early experimental work in the laboratory shows that upon passing a current through a proton-conducting solid electrolyte, the rate of methane dehydrogenation to ethane and ethylene can be enhanced up to 8 times the open-circuit rate at 750 °C over Ag electrodes. This research endeavor will be continued and completed with further electrocatalytic studies and more fundamental studies with electrode kinetics and electrolytic transport. The objective is to determine the

relationship between the ohmic-free potential and the reaction rate enhancement. Upon passing a current through an oxygen-ion-conducting solid electrolyte, methane conversion to synthesis gas was promoted with selectivities near 90% over Fe electrodes at 900 °C. It also appears that oxygen supplied through the electrolyte can be more selective than gaseous O_2. This research endeavor will be continued and completed by further examining the product selectivity and reaction kinetics on Fe in the presence or absence of H_2O vapor in the methane feed stream.

Molecular Modeling and Catalysis - By Design

Ames Laboratory
Iowa State University
Ames, IA 50011

154. Catalysis by Design

King, T.S.

Despite the widespread use of three-way catalysts, relatively little is known about the interaction between the metallic components. Synergistic effects occur when two metals are mixed together, and the effects are often attributed to two broad but incompletely understood principles termed geometric (or ensemble-size) and electronic effects. Also, structure sensitivity of the catalytic behavior is a factor in small metal particles, especially when one of the constituent elements preferentially segregates to various surface sites. These phenomena are intrinsically tied to the structure of the metal particles. This project will elucidate these effects by (1) theoretically predicting surface morphology, including site composition and micromixing of constituent metals, for small particles and single crystals as a function of reactive environments; (2) characterizing the surface of the supported metal particles in actual catalysts to confirm the utility of the theoretical predictions and to provide a basis for evaluation of catalytic behavior; (3) investigating the chemisorption behavior of various molecules on multimetallic single-crystal and supported-particle surfaces; and (4) correlating the catalytic behavior of well-characterized surfaces for the pertinent reactions with surface morphology.

Atlanta University
Atlanta, GA 30314

155. Hyperproduction and Secretion of Polyphenol Oxidase

Dashek, W.V.; Williams, A.L.

The objectives of this research are (1) to purify intracellular and extracellular polyphenol oxidases from *C. versicolor* maintained in liquid culture, (2) to determine if intracellular polyphenol oxidase is either *de novo* synthesized or activated from an intracellular precursor, and (3) to clone the gene and express it in *Escherichia coli*. The first approach is to establish the time courses for the appearance of two enzymes and to subsequently determine specific activities and to establish optimum growth conditions of the organism for maximum enzyme production, including determination of cofactor or inducer requirements. The second approach is to isolate the DNA or mRNA from the white rot fungus, use restriction endonucleases or cDNA methodologies to insert fungal genes into *E. coli*, and screen *E. coli* colonies for PPO production and secretion.

California Institute of Technology
Pasadena, CA 91109

156. Biocatalysis by Design: Predictive Models and Effects of Structure on Catalytic Properties

Goddard, W.A., III

A critical problem in the design of new biological catalysts is the limited current capability for prediction of the structure and properties of the new system. It is necessary to be able to predict secondary and tertiary structure on the basis of amino acid sequences (primary structure) because physical and chemical properties depend on the 3-D protein conformation. If the catalytic function and other properties of modified or synthetic enzymes could be predicted, a new biological system could be designed and synthesized to perform only those specific functions that are desired on the basis of structure and functional characteristics. Prediction of protein structure is being investigated by three approaches that combine random fluctuations with molecular dynamics to allow molecular forces to guide optimization of local structure. The first approach is full optimization, where a combination of molecular dynamics and random processes is used to search for energy minima of protein structures. Although only the amino acid sequences are required, several years of research and development are expected. The second approach is conformationally constrained optimization, where X-ray data places certain restraints on possible configurations. The third approach is NMR pair-constrained optimization, where NMR results further reduce the possible configurations that are feasible.

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

157. Catalysis by Design: Metal Clusters and Zeolite Catalysts

Bell, A.T.

The majority of industrially significant catalysts in current use are either zeolites or some kind of metal or metal oxide on an inert support. Although a large amount of research has been carried out on these catalysts, much of it is empirical, and catalyst evaluation and selection is still based upon extensive screening programs. The purpose of this project is to develop theoretical models that could be used to assist in the design of metal and zeolite catalysts. Quantum mechanical calculations will be carried out on the atomic-scale structure and catalytic properties of zeolites and mono- and bimetallic surfaces, and of the interactions of small organic molecules with catalytically active sites in zeolites and at metallic surfaces. Molecular

dynamics will be used to determine diffusion coefficients for molecules sorbed in zeolites, and dynamically corrected transition state theory will be used to describe the dynamics of desorption and reactive processes for both metals and zeolites. The results of all calculations will be validated by comparison with experimental measurements. The ultimate goal of the project is to assemble and integrate the individual elements of theory needed to describe the overall behavior of complete reaction networks.

158. Catalysis by Design: Novel Enzymes Using Catalytic Antibodies

Schultz, P.

Recently, antibodies have been found to be capable of acting as catalysts for a number of different reactions. Antibodies are proteins produced by animals in response to the deliberate or accidental injection of foreign molecules. Designing antibodies as catalysts is based upon the observation by Linus Pauling many years ago that "enzymes have high affinity for the transition state of molecules undergoing reactions, while antibodies have high affinity for molecules in their ground states." The procedure is to hypothesize what the transition state of the desired reaction would look like, synthesize a stable analogue of that transition state, use the stable analogue as an antigen to produce antibodies to the analogue, and examine these antibodies for catalytic activity. This can be done very easily now using the techniques of monoclonal antibody production. In this way, once created, the antibody-producing system can be stored frozen indefinitely, and the techniques of site-specific mutagenesis used to create minor changes in the antibody for structure–function studies. Catalytic antibodies (also known as "Abzymes") have been produced that catalyze the Diels–Alder reaction. This reaction, a fusion of a conjugated diene and an olefin to produce a six-membered ring, has not been observed in any natural enzyme system. This raises the possibility of designed catalysts for carrying out unusual reactions of economic significance with great specificity. The industrial partner for this project is Affymax Inc. The specific focus will be on enhancing the catalytic power of antibodies by allowing the substitution of chemically reactive and nonnatural amino acids and cofactors into their active sites. Computer models will be developed based upon experimental results and an understanding of the underlying science. They will be designed to predict the effect of amino acid substitutions and other modifications on enzyme stability, specificity, and activity.

Los Alamos National Laboratory
University of California
Los Alamos, NM 87545

159. Theoretical Studies of Hydrocarbon Catalysis on Zeolites

Hay, P.J.

The goal of this project is to develop computational tools to model chemical transformations of small hydrocarbon molecules within zeolite catalysts. The focus of this research is on the details of carbon–carbon bond formation within the pentasil zeolite, ZSM 5, for the conversion of methane to methanol. The modeling activity is to be complemented with an experimental program to provide validated modeling tools for industrial catalysts.

Pacific Northwest Laboratory
Richland, WA 99352

160. Periodic Ab Initio Hartree–Fock Theory/Site Isolation in Selective Alkane Oxidation

Hess, A.C.; Thompson, M.R.

The development of experimental and theoretical tools to study heterogeneous catalysis has been the focus of this effort. Research focuses on the development of novel solid-state formalism, its application to zeolites and clays, and experimental validation of molecular-level processes in commercial catalytic reactions. As part of the Catalysis-by-Design program, Pacific Northwest Laboratory (PNL) is pursuing the development of several tools aimed at facilitating the study of solid-state structure in heterogeneous catalysts. These include the development of periodic ab initio Hartree–Fock theory and its application to aluminosilicates and metal oxides, and the formulation of a model to describe the phenomena of "site isolation" in selective oxidation catalysts.

University of Pittsburgh
Pittsburgh, PA 15260

161. Theory of Biocatalysis: Electron Transfer Reactions

Beratan, D.N.

The principal project goal is the computer-aided design of enzyme biocatalysts with tailored catalytic rates. The focus of this project has been on electron-transfer enzymes, a major class of biological enzymes. In this project, a theory for protein electron tunneling pathway has been developed and implemented as computer models, which connect enzyme electronic structures and their reaction rates. Specific project objectives include (1) developing algorithms to map the key residues in proteins between electron-transfer sites that mediate electronic coupling and allow electron-transfer reactions to proceed; (2) identifying "hot" and "cold" spots with respect to electron transfer in native and modified proteins; (3) developing an understanding of primary, secondary, tertiary, and quaternary structural effects on electron-transfer rates; (4) using knowledge gained to stabilize energetic charge separated states and to enable the development of semisynthetic-modified protein energy conversion systems.

Sandia National Laboratories, Albuquerque
Albuquerque, NM 98195

162. Computer-Aided Molecular Design (CAMD) Methodologies

Shelmut, J.

Carbon dioxide represents a "free" source of carbon for the production of organic chemicals if suitable fixation catalysts can be devised. Reduction of carbon dioxide is an endothermic process, and the only free source of energy is solar energy as is used by plants in photosynthesis. If carbon dioxide could be activated it might react with the organic molecules and produce, for example, acetic acid by reaction with methane. The goal of this research project is to develop generic computer-aided molecular design (CAMD) methodologies and apply them to the design of a new generation of carbon dioxide activation catalysts. The CAMD effort will be guided by structural and chemical characterization of enzymes that activate and convert CO_2 to organic molecules. The biochemistry of CO_2 conversion has only recently reached a sufficient level of understanding so that the problem of mimicking the C1 catalysis of methanogens and other gas-metabolizing bacteria can be confronted. The ultimate objective of this project is a process for solar-driven "artificial methanogenesis".

Process Design and Analysis

National Renewable Energy Laboratory
Golden, CO 80401

163. Bioengineering Simulation Technology (BEST) Development

Wyman, C.

A government and industry consortium has been established at the National Renewable Energy Laboratory (NREL) to develop and integrate a series of computer programs to simulate process and unit operations in the bioprocessing area. A bioprocess model can be used to compare energy and economic benefits of various bioprocesses relative to conventional chemical processes, and to select the most efficient process of those assessed. At present, most new bioprocess designs are derived on the basis of the interests and technical capabilities of the proposer without due consideration of alternatives. For example, the fermentation process may be considered without the necessary study on product isolation. The purpose of this task will define process flowsheets for energy-efficient, cost-effective bioprocesses. The procedure will assist in selection of unit processes equipment and interconnections, identify important design parameters, and list alternatives to be considered. It will start with the BIOASPEN program, and modify and extend its operation. Participants in the consortium will have access to the program at NREL, receive instruction in its use, and receive programs and documentation for use in their own facilities.

Separations and Novel Chemical Processes

University of Hawaii
Honolulu, HI 96822

164. Product Recovery Using Reactions in Supercritical Solvents

Antal, M.

For this project, the recovery of products from dilute aqueous solution will be attempted by direct chemical reaction under supercritical conditions, such as 300 °C and 43 kg/mm^2 (1500 psi) in the presence of very dilute mineral acid. It has been shown that many organic compounds undergo an E_1 type of elimination reaction, and in a dilute aqueous solution ethanol is converted to ethylene, which separates from the water as soon as the pressure is released. Preliminary experiments have shown that similarly, n-butanol is dehydrated to a mixture of butene-1 and butene-2, with yields of 85%. Economic evaluations will be conducted and the conditions of dehydration optimized, with the main emphasis on the butanol and ethanol systems. After studies on synthetic mixtures, experiments will be conducted on actual fermentation broths to test out practicality and determine if any additional steps are necessary.

Idaho National Engineering Laboratory
Idaho Falls, ID 83415

165. Biological Extraction of Phosphate from Phosphate Ore

Rogers, R.D.

The phosphate industry uses about 316 x 10^{15} J/yr (0.3 quads/yr) for the separation of phosphate from apatite ore. This task is directed toward developing a bioprocess for solubilization and separation of phosphate from ore. The specific objectives of the research are (1) to define a microbiological system that will extract phosphate from its ore, (2) to develop a basic understanding of the biochemical mechanisms involved, and (3) to use modern biotechnology to develop a bioprocessing system for transfer to the phosphate industry. The approach will be to gain a thorough understanding of the biochemical interactions that cause the microbial release of phosphate from its ore. This will be accomplished by screening microorganisms obtained from areas of high phosphate content (i.e., phosphate mines, process waste streams, fertilized agricultural lands, and so forth) for their ability to solubilize phosphate. Research has shown that phosphate ore can be solubilized by a wide range of bacteria and fungi. Two organisms, one bacterial and one fungal, were selected for more detailed study and kinetic studies on ore solubilization are now completed. Laboratory-scale experiments are being conducted to determine whether batch or continuous operation is most efficient. Determination will be made of the necessity for separate production of the microorganism. Initial designs of a process and a pilot plant have been made.

Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

166. Separation by Reversible Chemical Association

King, C.J.

The objective of this project is to investigate and evaluate the use of reversible chemical association, or complexation, as a method for separating polar organic substances from dilute aqueous solution. Research will focus on (1) obtaining a sufficient understanding of underlying chemical, thermodynamic, and transport phenomena to enable rational selection of separating agents and methods of implementation and regeneration, as well as rational conceptual design and economic evaluation, and (2) improving processing technology, including novel methods for separation and regeneration. Current efforts include (1) identification, development and characterization of adsorbents and extractant capable of taking up carboxylic acids at pH substantially above the pK_a of the acid, yet capable of regeneration by means that do not involve chemicals consumption or waste production; (2) investigation of water-enhanced solvation of solutes of interest (acids, alcohols, and so forth) in hydrogen-acceptor solvents; and (3) implementation of regenerable complexation or chemical reaction for recovery of glycols, polyols, sugars, and/or hydroxycarboxylic acids from aqueous solution.

SENSORS AND CONTROLS

Advanced Sensors and Controls

Advanced Fuel Research, Inc.
East Hartford, CT 06108

167. A Rugged, Stable, FT-IR Interferometer for Process Monitoring

Solomon, P.R.

Innovative concepts are needed in advanced online sensors for application in industrial control systems leading to decreased energy consumption, better environmental control, better quality control, and increased productivity in U.S. industry. The goal of this research is to develop a vibration immune, rugged, permanently aligned, thermally stable, low-cost Fourier transform (FT) mid-IR absorption spectrometer for process and environmental monitoring. The innovation in this system is an advanced and novel dynamically balanced "isolation interferometer" with corner cube optics in which the mirror motion is decoupled from external vibrations. In Phase I of the project, an isolation interferometer was developed that demonstrated the ability to reduce external vibrations. Phase II, currently in progress, is to design, construct, and test a complete FT-IR absorption spectrometer incorporating the corner cube isolation interferometer and other advanced components for applications in process and environmental monitoring. Some applications include combustion diagnostics, continuous emission monitoring of smoke stacks, auto emission testing, medical diagnostics, and ambient air monitoring.

168. In Situ FT-IR Monitoring of a Black Liquor Recovery Boiler

Solomon, P.R.

The purpose of this project is to develop and test a rugged, commercial Fourier transform-infrared (FT-IR) spectrometer based on an advanced vibration immune instrument for operating and analyzing data in black liquor recovery boilers as well as to develop control strategies for improving boiler performance and emission levels based on these measurements. The application of this technology for online monitoring of recovery boilers could lead (1) to better understanding of the processes occurring in the boiler, (2) to technology for online monitoring and control, and (3) to data for the development and validation of recovery boiler models. The first in situ diagnostics within an operating black liquor recovery boiler using FT-IR emission and transmission spectroscopy have been successfully performed. In addition, the use of FT-IR tomography to convert multiple lines-of-sight into spatially resolved data and the measurement of emissivity, temperature, and physical properties of surfaces has been demonstrated for the first time.

Babcock & Wilcox Company
Alliance, OH 44601
Research and Development Division

169. Development of an Online Sensor for the Measurement of Lignin Concentration in Wood Pulp

Berthold, J.W.; Jeffers, L.A.; Roman, G.W.

The objective of this project is to develop a sensor that measures the concentration of lignin in wood pulp, online and in real time. The sensor will be based on laser excited fluorescence and will not require sample extraction or sample preparation. It will be configured to provide feedback control to the digester as well as feedforward control to the bleach plant. Controlling the concentration of lignin in wood pulp is crucial to the amount of energy consumed by the digester, the quantity of bleach used after the digestion process, and to the product yield and quality. This translates into energy conservation, economic savings, and reduction of downstream pollutants. The sensor being developed will be nonintrusive and operate continuously, making real-time control possible. This initial investigation was performed on northern spruce and southern pine pulp samples and included specimens with KAPPA numbers ranging from 15 to 60. The current research effort is concentrating on testing additional wood species, a broader range of KAPPA numbers (3 to 100), and is also investigating the effect of black liquor on the fluorescence spectra. Once the current research efforts have been completed, a prototype sensor will be designed and constructed. This prototype sensor will be refined during laboratory testing and will then be field tested in an operating pulp mill to verify its operation in a mill environment.

Energy and Environmental Research Corporation
Irvine, CA 92718

170. Glass Temperature Sensor

Koppang, R.R.

The objective of this project is to develop an advanced noncontacting temperature sensor to be employed for use in a thermal analysis system for glass furnaces to an accuracy of ±1 °C. A lab furnace has been built and test data will be collected for verification of previous calculations and inclusion of data in the control computer algorithm. Field tests of the sensor will be completed by midsummer 1993.

University of Florida
Gainesville, FL 32611
Department of Chemical Engineering

171. Characterization of Physical Properties of Kraft Black Liquor

Fricke, A.L.

The project objective is to develop methods for measurement of rheological, thermal, and surface properties of black liquor, and to develop or improve methods for chemical analysis of black liquor and for molecular characterization of lignin. Results to date demonstrate that the lignin polymer dominates high solids behavior and the properties can be reduced and correlated by methods based on polymer theory and/or dynamics. These results represent the first (1) reliable rheological data as a function of solids, temperature, and shear rate; (2) successful correlation of heat capacity at all solids and temperature; (3) quantitative determination of heats of dilution for black liquor solids; (4) determination of enthalpy-concentration relations; (5) determinations of vapor pressure equilibria for black liquors over an extensive range of solids concentration and pressure; (6) determinations of density and thermal expansion at solids concentrations up to 100%; (7) demonstration of thermodynamic consistency of thermal and vapor pressure data; (8) accurate determination of M_n and M_w of lignins; (9) statistical evaluation of M_w of lignin with pulping conditions; (10) universal correlations for viscosity as a function of solids concentrations, temperature, and shear rate for temperatures up to 140 C and solids concentrations up to 85%; and (11) relation of black liquor solids composition to pulping conditions for slash pine. The final expected products of the program are a large data bank and a set of correlations to be used to predict liquor physical properties from liquor composition or pulping conditions for design or design improvements of recovery systems.

Guided Wave, Inc.
El Dorado Hills, CA 95630

172. Thin-Film Device for Process Measurement: Phase III Industrial Test

Goldman, D.S.

Phase III of the development of a compact analytical device, based on thin-film optical waveguide technology, for online chemical analysis of complex process fluids is evaluating industrial test strategies for chemical and petrochemical application. Prototype devices for visible and near-IR frequencies, and a test flow cell have been developed. The advantage of this technology is its ability to examine light-scattering mixtures quickly and without separation costs and delays. The sample is "sensed" within a micron of the surface of an internal reflectance element at each reflection without transmitting light across a volume of sample. Thin films, less than 1-μm thick are used allowing thousands of internal reflections to occur that interact with the liquid. Complex fluid samples from industry were solicited and tested. White (TiO_2) and black (activated carbon) slurries containing organic and aqueous–organic materials were successfully characterized without any adverse spectral effects from the suspended particles. A set of activated carbon slurries was tested and the device was able to distinguish between samples having slightly different hydroxyl contents in the methyl ester mix. This demonstration illustrates the application of the sensors to fluids where normal light transmission is not possible and separation techniques may be either too slow or costly, for example, characterization of crude oils, polymers, or catalytic reactor performance. In addition to the industrial test, a prototype probe will be developed to advance the sensor to an inline device not requiring a slip stream.

Institute of Paper Science and Technology (IPST)
Atlanta, GA 30318
Engineering and Paper Materials Division

173. On-Machine Sensors to Measure Paper Mechanical Properties

Hall, M.S.; Brodeur, P.H.

The measurement of the velocity of ultrasound provides a nondestructive technique to determine the elastic stiffnesses of paper. These mechanical properties are very sensitive to paper machine process variables and also are highly correlated with paper end use performance. The immediate objective is to develop sensors capable of measuring the velocity of ultrasound in the in-plane and thickness directions of paper while the paper is moving at line speed on the paper machine. The goal is to obtain a continuous record of product quality and to provide the data for controlling the papermaking process. Currently, efforts are placed establishing a working relationship with a vendor of instrumentation and control systems for paper machines. Prototype sensors and electronics will be built and evaluated in the laboratory in preparation for testing on a paper machine at a host mill test site. Successful online implementation of this instrumentation will permit energy savings by optimization of energy intensive processes and avoid waste by minimizing substandard production.

Oak Ridge National Laboratory
Oak Ridge, TN 37831

174. Online Sensor for Magnesium Production

Young, J.P.

The objective of this project is to develop sensors to measure the concentration of magnesium ions, fluoride ions, and impurities in magnesium molten salt bath and alumina concentration in molten cryolite baths for Hall–Heroult cells. Researchers will use Raman studies to determine chemical species in the bath.

Pen Kem, Inc.
Bedford Hills, NY 10507

175. Development of Laboratory and Process Sensors to Monitor Particle Size Distribution of Industrial Slurries

Pendse, H.P.

In 1988, a cooperative research program was undertaken to develop laboratory and online PSD sensors to monitor industrial slurries without dilution, addressing the submicron particle population, with rapid response capability. In this project one online and two laboratory prototypes have been built and evaluated in the titanium dioxide manufacturing facility at the Du Pont plant over a three month period. The sensor proved to be robust, and provided reproducible data that were sensitive to changes in processing conditions. The PSD sensor development project has resulted in successful technology and prototypes that form the basis of a commercial instrument currently under development. Further work is under way on active ultrasonic spectroscopy for simultaneous size and shape analysis. Other potential applications include use of ultrasonic spectroscopy for monitoring coating formulations used in papermaking.

University of Tennessee at Knoxville
Knoxville, TN 37996
Measurement & Control Engineering Center

176. Development of an Online Chemical Composition Analyzer

Garrison, A.A.; Moore, C.F.; Roberts, M.J.

The development of an online Raman spectrometer system for chemical composition determination in distillation environments is completing the industrial testing phase at the Tennessee Eastman Corporation in Kingsport, Tennessee. The prototype sensor system has been installed on a bottoms product recovery column and is currently being tested. The Raman spectrum of a mixture from an internal stage of a distillation column has been obtained using a test cell, and 35-m fiber-optic extension cables, with a good spectral signal-to-noise ratio. An empirical mathematical model based on correlation between the spectral features and the composition has been developed that provides a root-mean-square uncertainty of less than 2% in the data analysis. Static and dynamic modeling of the distillation column before and after sensor installation are providing a total systems approach to utilizing internal chemical composition data for improved control. The goal of the project is to lower distillation column energy use and increase product throughput by improved control.

SEPARATIONS

Separation Systems

Battelle Columbus Laboratories
Columbus, OH 43224

177. Improved Electroacoustic Dewatering Belt Press for Food

Chauhan, S.P.

The objective of this project is to develop and test an enhanced prototype device to demonstrate the electroacoustic dewatering concept for a food material (corn fiber), optimize the process, and disseminate the results to promote commercial adaptation of the technology. Phases I and II, now complete, proved the technical feasibility of the concept at laboratory scale and then concentrated on design modifications of larger scale dewatering units. Phase III, currently in progress, has made modifications to a commercial 1-m belt press. Initial shakedown tests at the press manufacturer have shown the need for additional modifications to the belt design and construction. Field tests at a food processor will follow the modifications to the belt.

Georgia Institute of Technology
Atlanta, GA 30332

178. Sensor System to Monitor Nitrogen Transfer from Agricultural Cropland

Walsh, J.L., Jr.

The project objective is to develop an integrated-optics (IO) sensor capable of measuring gaseous ammonia concentrations in the range of 100-ppb. The sensor can then be used to measure the losses from agricultural croplands after the application of nitrogen fertilizers. The IO sensor could be installed on an anhydrous ammonia fertilizer applicator and used to control the application rate and depth settings of the applicator. The sensor could also be used to measure the loss of nitrogen after the application of a urea-based fertilizer to determine the need for additional fertilizer application. The project will consist of two phases. During Phase I, an IO sensor will be developed and tested using a soil simulator test bed. Upon successful completion of Phase I, a Phase II field testing program will be initiated to determine the performance of the IO sensor system under actual field conditions. The project will be conducted by a joint team of investigators from the University System of the State of Georgia. The sensor development will be the responsibility of the Georgia Tech Research Institute at the Georgia Institute of Technology. The field testing will be the responsibility of the Griffin Georgia Agricultural Experiment Station of the University of Georgia.

Idaho National Engineering Laboratory
EG&G Idaho, Inc.
Idaho Falls, ID 83415

179. Sonic Sensor System

Beller, L.S.

The objective of this project is to develop a laboratory prototype sensor to determine the interior temperatures of particulate foodstuff during processing. The project uses speed-of-sound tomography as a noninvasive method of internal temperature measurement. The concept is expected to save a minimum of 11 x 10^{15} J/yr (1 x 10^{13} Btu/yr); solve a product waste disposal problem; reduce operating costs by eliminating punctured food cans and other containers; and permit the widespread use of aseptic selected food materials, the requirements of the tomographic process; and design approaches for the ultrasonic sensor. The process was shown to be technically feasible. Phase II is well under way with the objectives of developing a prototype system.

National Food Processors Association
Oakland, CA 94568

180. Sonic Temperature Sensor Development

Kimball, R.N.

This project supports the sonic tomography project being researched by Idaho National Engineering Laboratory (INEL), and provides guidance and data about the operation of the food industry. The prototype sensor system will be tested in the National Food Processors Association (NFPA) pilot plant.

Purdue University
West Lafayette, IN 47907
Department of Agricultural Engineering

181. Crop Ripeness Sensor

Krutz, G.W.

Nuclear Magnetic Resonance (NMR) spectroscopy is recognized as one of the most powerful techniques for chemical analysis. The NMR spectrometer provides an accurate and nondestructive method of determining chemical structures in liquid and solid materials. The main goal of this project is to investigate the possibility of developing a low-cost NMR-based sensor to determine the ripeness (i.e., sucrose content) of fruit. Improved monitoring of ripeness of fruits and vegetables from production to distribution could be achieved by using the proper sensors. This would provide high-quality and value-added products for both distributors and consumers. With improved sensors, production costs could be reduced and more effective processing standards and controls could be implemented.

Southwest Research Institute
San Antonio, TX 78284
Department of Electronics and Physics

182. Development of a Hydrogen Transient Nuclear Magnetic Resonance Sensor for Moisture Measurement

Nicholls, C.I.

The objective of this project is to develop a hydrogen transient nuclear magnetic resonance (HTNMR) sensor that monitors the moisture content of materials being dried, minimizing drying energy requirements and maximizing process efficiency. Emphasis is on applications involving the drying of processed agricultural products such as corn, wheat, maize, and soybeans as they are converted into commercial items such as animal feed, starch, grain proteins, flour, and so forth. This project involves HTNMR sensor development with eventual commercialization of the process. Phase I involves developing the sensor concept and investigating its feasibility, developing the sensor system, and verifying the technical and economic feasibility of the sensor.

TECOGEN, Inc.
Waltham, MA 02254

183. Superheated Steam Atmosphere Drying with Exhaust Recompression

DiBella, F.

For the thermal drying processes where water is to be removed via evaporation from the feedstock, attempts have been made to reduce the consumption of energy using exhaust waste heat recovery techniques, improved dryer designs, or even the deployment of advanced mechanical dewatering techniques. Despite these efforts, a large amount of thermal energy is still lost because the latent heat of evaporation is not recovered from the evaporated water. The objective of this project is to establish the feasibility of using a superheated steam atmosphere for drying granular material. TECOGEN, Inc. is developing a steam-atmosphere dryer system that provides the means for recovering this latent heat, thus significantly increasing the dryer's thermal efficiency. The advanced concept uses a unique drying chamber design that is integrated with a steam recompression system. The use of this novel drying chamber design is thought to be a major contribution to the science and art of drying. Thermodynamic analysis has projected that the drying energy requirements for the integrated system using the new dryer plus steam recompression can be reduced by as much as 50% over present air dryers. This energy reduction is accomplished by allowing the evaporated feedstock's latent heat content to be directly returned to the drying chamber.

MATERIALS PROCESSING

Foundry Technology

American Foundrymens' Society
Des Plains, IL 60016

184. Online Process Modeling of a Cupola Furnace
Twarog, D.L.

The project objective is to develop a model to optimize the process control and the efficiency of the cupola furnace as a foundry melting unit. The process model would permit control of cupola operation in order to meet the desired product quality with optimum efficiency and permit menu driven, user friendly, offline studies to be made for determining process and cost impacts of intended changes in process inputs. The work involved consists of a critical review of literature and information available on existing cupola and blast furnace models to apply available technology. Thermochemical and kinetic databases will be developed and a critical review of currently available sensors will be performed to recommend sensor development activity not included in the scope. Conceptual models of heat transfer-fluid flow and heat and mass balances will be developed including equation statements. Industry review will be obtained prior to verification of the model with operational data to compare computational results with actual cupola data. An expert system scoping study will be conducted to integrate the cupola model into a broader foundry model. The results will be discussed with the foundry community.

185. Development of Precision Evaporative Casting Technology
Twarog, D.L.

The project objective is to further develop and optimize Evaporative Pattern Casting (EPC) technology for a broad based application. Sand flow and compaction will be evaluated. Factors that influence the dimensional precision of castings produced via the EPC process will be evaluated. Critical process parameters and system properties that control the dimensional precision of the evaporative casting process will be identified. Compaction of granular materials, heat transfer, thermodynamics, casting defect detection by various methods, refractoriness of coating materials, dimensional analysis, glue formations, and principles of vibration compacting are involved.

Argonne National Laboratory
Argonne, IL 60439

186. Casting Modeling
Sha, W.T.

The purpose of this project is to develop state-of-the-art computer software for simulating the materials casting process. The COMMIX thermal-hydraulics code, previously developed under DOE sponsorship, will serve as the basis for this software development to predict mold filling and solidification of cast materials. The costs of mold design will be reduced through the prediction of the mold filling and temperature distribution, natural convection and solidification, gas entrapment, and premature freezing. Energy will be saved through reduced materials melting requirements, reduced scrap, and reduced environmental operating costs. An energy savings of approximately 46 billion joules (44 million Btu) annually is possible.

Glass

Vortec Corporation
Collegeville, PA 19426

187. Research and Development of a Rapid Glass Refiner
Bartone, L.M., Jr.

The objective of this project is to develop an advanced rapid glass refining system that can be applied to both conventional and advanced glass melting furnaces to increase the productivity of and improve the energy efficiency of glass melting furnace systems. The quality goals for the glass produced by the rapid refiner include blister-free glass with <1 seed/gram for container glass and <7 seeds/100 grams for flat glass applications. Batch tests on an 18,000 kg/day (20 ton/day) unit will be completed in 1993.

Metals Initiative

ARMCO, Inc.
Middletown, OH 45043
Research & Technology Division

188. Direct Strip Casting of Low-Carbon Steel
Sussman, R.C.

The objective of this project is to establish the technical and economic feasibility of casting a low-carbon steel sheet on a single-wheel caster utilizing the open channel process. Efforts are focused on (1) casting approximately 180 heats of steel ranging from 227 to 1361 kilograms (500 to 3000 pounds) to produce a steel strip on a single-wheel caster; (2) developing mathematical models of heat transfer and solidification, fluid flow through tundishes and nozzles, and performing a parametric study of the casting variables; (3) developing process improvements including pouring box heating, sensor development, and electromagnetic containment; (4) performing refractory studies; (5)

performing material studies on as-cast and finished strips; and (6) providing technical and economic assessments of the direct strip casting process, and conceptual and budgetary engineering for a pilot plant. Implementing the direct strip casting process would eliminate the need for reheat furnaces and hot strip mills. The energy savings associated with this technology are estimated to be 14 x 10^{16} joules per year (0.13 quadrillion Btu/year), reducing operating costs by approximately $43/ton compared to conventional operating practices. Nonenergy savings include a reduction in CO_2 emissions by 19 billion kilograms/year (21 million tons/year) and NO_x emissions by 16 billion kilograms/year (18 million tons/year).

American Iron and Steel Institute
Pittsburgh, PA 15235

189. Development of Direct Steelmaking

Aukrust, E.

This project is part of the Metals Initiative, the goal of which is to develop energy-efficient steel processes. The purpose of the direct steelmaking project is to develop an energy-efficient, economically competitive, continuous process that derives at least part of its advantages from the elimination of coke and the high capital requirements and environmental problems associated with coke ovens. The advantages of such a process would be (1) more effective use of domestic raw materials; (2) continuous, rather than batch, operation; (3) elimination of coke and its associated environmental problems; (4) ease of start-up and shutdown; and (5) modular design, which will facilitate rapid technology transfer and incremental adjustments in capacity and thus easy adaption to market conditions. The experimental work in this project includes five main areas: (1) laboratory studies on the physical and chemical phenomena of smelting and refining steel; (2) laboratory experimental work on postcombustion and heat and mass transfer; (3) laboratory and pilot-scale prereduction of hematite (Fe_2O_3) pellets to wustite (FeO); (4) smelting and refining in a pilot-scale smelter at Universal, Pennsylvania; and (5) postcombustion in large-scale steelmaking trials.

190. Advanced Process Control Research Program for the Steel Industry

Kavanagh, L.

The objective of this program is to design, test, and commercialize selected sensors, control devices, and software for steelmaking, casting, rolling, and coating operations. The program consists of six projects in four areas: (1) primary steelmaking, (2) continuous casting, (3) rolling and annealing, and (4) coated products. If successful, these projects could save 15 x 10_{15} joules each year (0.014 quadrillion Btu/year) and reduce operating cost by approximately $315 million annually. Each of the six projects is organized with a research partner to perform the work, a sponsoring steel company to guide and demonstrate the research, and a commercialization partner to manufacture and sell the project's development. This organizational structure should lead to rapid commercialization of successful developments.

Argonne National Laboratory
Argonne, IL 60439

191. Electrochemical Dezincing of Steel Scrap

Dudek, F.

The objective of this project is to build and operate a pilot plant to demonstrate a two-step process for the continuous dezincing of steel scrap. The products from this process will be clean, dezinced steel scrap and metallic zinc. A scrap dezincing process will save the nation approximately 53 x 10^{15} joules per year (50 trillion Btu/year), and reduce raw material costs by $160 million per year. In addition, the process provides some environmental benefits such as increasing the recyclability of steelmaking fume and eliminating zinc from wastewater streams.

Lawrence Livermore National Laboratory
University of California
Livermore, CA 94550
Engineering Sciences Division

192. Superplastic Steel Processing

Landingham, R.

The objective of this project is to develop and demonstrate a process for the manufacture of superplastic ultrahigh carbon steel alloys. Efforts are focused in four areas: (1) identifying alloys' forming and casting properties, (2) determining applications and identifying parts for forming, (3) designing dies and forging of parts, and (4) developing industrial scale casting practices. Assuming production levels of 2 billion kilograms/year (2 million tons/year), the energy savings by implementing superplastic steel are estimated to be approximately 11 x 10^{15} joules/year (0.01 quadrillion Btu/year). Manufacturing costs could be reduced by 17% for forging and machining operations.

Lehigh University
Bethlehem, PA 18015

193. Rapid Analysis of Molten Metals Using Laser-Produced Plasmas

Kim, Y.W.

The objective of this project is to develop a sensor probe to rapidly determine the chemical composition of molten iron and steel using spectroscopic analysis of laser produced plasmas. Prototype units will be tested in two different steelmaking plants. This technology is applicable to a wide range of solid and liquid metals. Widespread implementation of this probe by the carbon steel industry could save approximately 11 x 10^{15} joules/year (10 trillion Btu/year) and reduce operating costs by $488 million annually.

National Institute of Standards and Technology, Gaithersburg
Gaithersburg, MD 20899

194. Intelligent Processing of Rapidly Solidified Metal Powders by Inert Gas Atomization

Pugh, N.

The objective of this project is to develop an intelligent processing system that will permit online control of the particle size distribution of rapidly solidified metal powders. Efforts will focus on (1) demonstrating real-time particle size sensing; (2) designing, building, and evaluating fluid-flow sensors; (3) developing material properties for Alloy 625; (4) developing a computational fluid dynamic model; (5) fabricating process control hardware; and (6) demonstrating control strategies. Energy- and cost-savings analysis will be provided because many powder production processes obtain 50% or less yield due to suboptimal particle size distributions. Application of existing industrial power-producing facilities will enable a reduction in the Gaussian distribution of particle sizes, thus increasing yield.

Weirton Steel Corporation
Weirton, WV 26062

195. Integrated Manufacturing Information System

Murphy, W.

The objective of this project is to develop a material management system for inventorying cold rolled steel coils. This system incorporates real-time tracking of the coils during and after rolling, and continuous integration with production, scheduling, customer orders, and inventory strategies. Up to 30,000 different coils can be present within a steel mill at any given time, varying only by the different rolling, annealing, trimming, coating, and wrapping processes. Losses from excessive coil handling, replacing damaged coils, and idle processing lines is in excess of $2.78/metric ton ($3/ton). One solution currently being examined is the use of a radio transmitter attached to the individual coils. These transmitters will periodically broadcast identifying information, and through triangulation techniques, the location of each coil can be monitored.

Process Electrolysis

Alcoa Laboratories
Alcoa Center, PA 15069
Armor Systems Development

196. Low-Temperature Electrolysis of Alumina

LaCamera, A.F.

The objective of this project is to assess the commercial viability of high surface area anodes (HSAA) and a low-temperature electrolyte in aluminum reduction cells. Goals include inert HSAA corrosion rates that result in commercial-purity aluminum, and economically viable anode live and cell performance. Deliverables sought are a 125-kA retrofit cell design with a 20% specific energy reduction and the determination, at pilot scale, that using HSAA and a low-temperature molten salt is technically viable and sufficiently attractive to achieve commercial implementation.

Dow Chemical Company
Midland, MI 48640

197. Inert Ceramic Anode for Magnesium Production

Brubaker, B.D.

Contemporary ceramic science and engineering will be applied in a four-year project, with go–no-go decisions after the first two phases, to the fabrication of an inert ceramic anode for increased energy efficiency in electrolytic magnesium production. The objective of the first of three phases (in progress) is to fabricate crack-free anodes capable of low-wear rates in a 7 to 10 d laboratory operation. The objective of Phase II is to demonstrate a six-month lifetime of a full-scale inert anode with electrical performance equal to a new graphite anode in a commercial magnesium production cell.

EMEC
New Kensington, PA 15068

198. Electrolysis of Neodymium Oxide

Keller, R.

The objective of this project is to develop an electrolytic process for the continuous and economic production of neodymium metal and neodymium alloys from neodymium oxide. Phase I, currently in progress, is to select an efficient electrolyte for operation (electrical conductivity, and metal and oxide solubilities) relatively free of envisioned problems (anode effect and cathode scum), and to perform an economic and energy-savings assessment of the process and the end-use motor applications. If continuation is warranted, Phase II will verify technical feasibility at laboratory scale, and Phase III will provide a proof-of-concept for this technology at the pilot scale.

Metalor USA Refining Corporation
North Attleboro, MA 02761

199. Fluidized Bed Electrowinning of Copper

Kinneberg, D.J.

The objective of this project is to show that fluidized bed electrowinning (recovery of metals from solution by electrolysis) is viable for industrial operations through design, construction, and operation of a 10-kA fluidized bed copper-producing electrolytic cell. This technology is to be transferred to others through licensing agreements.

Pacific Northwest Laboratory
Richland, WA 99352

200. Development of Inert Electrodes for Aluminum

Windisch, C.F.

The objective of the scaleup activities is to perform the required research and development of fabrication methods for large anodes and to test the large units in a cell that represents sections of a commercial unit. The approach will be to allow the Pacific Northwest Laboratory (PNL) to perform the required critical path activities while cost-share research is pursued with industry through solicitation. Solicitations will cover both material fabrication and cell application. Results should provide the industry with viable methods for anode manufacture and application.

Reynolds Metals Co.
Richmond, VA 23225

201. Field Testing of Titanium Diboride Cathodes in Commercial Aluminum Cells

Richards, N.

The project objective is to determine the technical and economic viability of graphite-containing titanium diboride materials in low-cost shapes for use as cathodes in aluminum electrolytic cells in an effort to stimulate subsequent demonstration and commercial application. Included are (1) mathematical models for the prediction of cost-reduction cathode shapes, (2) determination of optimum electrode area ratios, (3) voltage reduction and effect on current efficiency by reduced anode–cathode distance, (4) production of cathode shapes using proprietary material processing technologies, (5) commercial and pilot cell operation for data acquisition and cathode longevity determinations, (6) analysis of as-fabricated and as-tested cathodes, (7) failure mechanism evaluation, (8) development of cathode holder–anode stops, and (9) assessment of energy savings and technical–economic viability.

Refractories

Aluminum Company of America
Alcoa Center, PA 15069
Alcoa Technical Center

202. Lightweight Refractory Aggregates

Pearson, A.

The objective of this project is to develop a lightweight, high-temperature, aggregate for use in a variety of high-performance insulating refractory applications. Application of these aggregates in the aluminum, glass, cement, and iron and steel industries will significantly decrease energy consumption and will increase domestic end-user industry competitiveness. The established project goals are to produce an alumina-based aggregate with 30% less bulk density, with at least 80% of current aggregate crushing strength, and with costs not to exceed existing alumina aggregates by more than 25%.

Schuller
Littleton, OH 80127

203. Development of High-Performance Refractory Fibers with Enhanced Insulating Properties and Longer Service Lifetimes

Martin, P.C.

The objective of this project is to develop improved high-performance refractory fibers with higher service temperature and lower shrinkage properties than existing fibers in order to enhance insulating properties and lengthen service times. Application of these fibers in the aluminum, glass, cement, and iron and steel industries will significantly decrease energy consumption and increase domestic end-user industrial competitiveness.

SMALL BUSINESS INNOVATIVE RESEARCH

Small Business Innovative Research

Advanced Technology Materials, Inc.
Danbury, CT 06810

204. A Real-Time X-Ray Detector
Kurtz, D.

In situ monitoring of critical material properties would greatly enhance process control of a wide variety of manufacturing technologies. Position-sensitive fiber optic X-ray scintillation detectors (PSSD) can be used to simultaneously measure several critical solid polycrystalline material parameters such as thickness, crystal structure, crystal perfection, preferred orientation, and residual stress. Compared with traditional X-ray detectors, the PSSD system is very compact; requires no scanning; and, most importantly, has very rapid sampling time (≤1-sec). All these attributes make it ideally suited for real-time analysis. Phase I of this project addresses the development of a real-time X-ray detector for use in harsh environment coating systems. In Phase II, the PSSD X-ray monitor will be incorporated into manufacturing processes for feedback process control.

Caldon, Inc.
Pittsburgh, PA 15216

205. Measurement of Pulverized Coal and Primary Air Flow to Individual Burners of Industrial and Utility Boilers
Archer, D.H.

In the operation of large industrial and utility boilers, variability in the flow of pulverized coal and air infeed pipes results in flames from the multiple, individual burners that vary in the temperature, shape, and composition of the combustion products, including excess oxygen (O_2), nitrogen oxides (NO_x), carbon monoxide (CO), and unburned hydrocarbons. Large imbalances in coal and air flows among burners can lead to such significant boiler operating problems as reduced steam production; increased energy losses in the heat of the stack gases and the carbon of the ash; decreased boiler efficiency; boiler tube wastage; an increased potential for leaks, increased slagging, and ash deposition; and excessive emissions of NO_x, CO, or unburned hydrocarbons. In this program, a team of small businesses is developing, demonstrating, and evaluating a system composed of ultrasonic coal and air flow instrumentation together with manual adjustments or automatic controls to maintain balance among coal and air flows to boiler burners. This system helps boiler operators achieve uniform flames over the full range of operating conditions, thus providing for enhanced boiler capacity, efficiency, and availability, as well as reduced emissions. In Phase I, a functional specification is being provided for this system, as well as a preliminary design or specification of the hardware and software and a statement of its cost and benefits. A site and a cooperating utility or industrial organization will be identified for a prototype demonstration. Phase II will include the detailed planning and design of the demonstration, fabrication of the test hardware and software, and installation and operation of the system at the cooperating site.

Chromex, Inc.
Albuquerque, NM 87107

206. A Rugged, Online, Multiple-Input Fiber Optic-Based Raman Sensor for Industrial Process and Monitoring Control
Bret, G.G.

Research in this project is being conducted to develop a compact, rugged, online, multiple input, fiber-optic-based Raman process monitoring and control sensor capable of operating in harsh industrial environments. Charge-coupled device array detector-based Raman spectroscopy, employing laser diodes and optical fiber probes, capable of sensitivities comparable to or better than the Fourier transform Raman method, has already been demonstrated. This new multiple input online sensor can probably be implemented in a sealed, compact, and rugged instrument having no moving parts. The instrument being studied in Phase I is based on an existing 100-mm f/2 imaging spectrograph design that, because of its high throughput and imaging capability, is capable of simultaneously monitoring and controlling a number of input spectral channels. The instrument has a high signal-to-noise ratio, which promises to make the method a true trace detection technique. Theoretical arguments supported by experimental results show that it is reasonable to anticipate a compact, rugged (even portable), multiple input Raman system capable of convenient and rapid multipoint detection and quantification of analyses in process environments.

Ciencia, Inc.
West Hartford, CT 06108

207. An Advanced Fluorescence Sensor for Process Control
Fernandez, S.M.

The development of an advanced frequency-agile sensor for online chemical analysis of fluorescent species in process streams is the objective of this project. This sensor is based on the innovative use of tunable acoustooptic filters to achieve random-access wavelength selection with microsecond switching time, high optical throughput for

enhanced sensitivity, and high spectral resolution for accurate measurements with high background discrimination. The sensor will be compact, rugged, and suitable for deployment in harsh industrial environments. In Phase I, a rugged prototype device is being built and tested by monitoring a model organic compound. If successful, the proposed technology will bring to online, real-time sensing, sophisticated spectral analysis now available only offsite in the laboratory with a very slow turnaround time for results.

Cushing Associates, Inc.
Annapolis, MD 21401

208. A Comprehensive Flowmeter for All Materials

Cushing, V.J.

It has long been established theoretically and experimentally that performance of the electromagnetic (EM) flowmeter does not, in principle, depend on any constitutive property of the metered material. It therefore holds promise of metering any material that can be blown, pumped, or extruded through a pipe. To date, the principal practical problem with the EM flowmeter involves the tradeoff that must be made to extract the flow signal while discriminating against triboelectric noise (when the measurand is an insulator) and/or zero-point drift (a spurious signal) when the magnet frequency is above the triboelectric noise spectrum. The EM flowmeter operates unequivocally as a volumetric flowmeter; by utilizing the Clausius–Mossotti relationship for insulating materials, it operates optionally as a mass flowmeter for measurands in the solid, liquid, or vapor phases, or any combination thereof. In light of today's capability in digital signal conditioning, it appears feasible, using a square-wave magnetic induction, to ascertain at all times (1) the true flow signal and (2) the spurious, drift signal. Phase I will demonstrate this by obtaining EM flowmeter flow signal data, digitizing and storing it, and carrying out the discriminating digital process with a 486-class microcomputer. The achievements of the Phase I effort should result in the design of a dedicated digital signal conditioner, operating in real time, to enable EM flowmetering of any material.

Defense Research Technologies, Inc.
Rockville, MD 20850

209. Development of an Oxygen Sensor for Continuous Measurement in Molten Steel

Phillipi, R.

This effort is directed toward the development of a continuous reading oxygen sensor for liquid steel service. Although well known as a critical parameter in the energy-efficient production of quality steel, oxygen content is currently measured using a disposable zirconia sensor capable of only intermittent operation. Despite the fact that fundamentally nothing has precluded the use of such a zirconia based sensor for continuous determination of oxygen content, two major obstacles have prevented this important technical advance. First, the simultaneous and continuous temperature measurement required by the zirconia cell was never available; second, zirconia is very sensitive to thermal shock. Overcoming these obstacles requires the use of spin-off technology from earlier efforts that led to a shock-resistant continuous temperature measurement device suitable for steel mill service. In Phase I, a robust zirconia cell with an ablative cap is being designed, fabricated, and iteratively tested until a configuration capable of direct immersion is achieved. The recently developed continuous temperature measurement technology will then be adapted for close proximity measurement to the zirconia cell. The steel oxygen content is determined when electromagnetic force and temperature are measured simultaneously and a known oxygen content reference material (typically chrome/chrome oxide) is placed in contact with the zirconia cell.

Dexter Research Center, Inc.
Dexter, MI 48130

210. Multiplexed Thermopile-Based IR Imaging Arrays

Toth, R.

This project investigates the development of thermopile-based IR imagers using silicon integrated-circuit technology and state-of-the-art micromachining. The devices should permit the remote monitoring of temperature and temperature uniformity in furnaces and other process facilities for which contact measurements are not possible. The project also provides the key element in advanced thermal sensing systems capable of automatic compensation for device offsets and nonlinearities as well as object emissivity variations. Building on research performed at the University of Michigan, the work focuses on transferring that technology to a commercial product. In Phase I of this project, the University's previous research vehicle, a 32-element linear imager, is being redesigned to make it more compatible with foundry fabrication and to optimize it further for specific applications. Micromachining capabilities are being installed so that eventual production wafers, when returned from the foundry, can be etched in-house as the final step in the process to create the finished imagers. In addition, a package that preserves the high performance of the detector, and is consistent with high production volumes at low cost, is being developed. Finally, prototype arrays fabricated at the University are being tested to determine their performance. Phase II would initiate imager wafer fabrication at a commercial foundry and explore practical wafer performance and yield in high volumes. It would also investigate full area arrays based on this technology.

Direct Measurement Corporation
Longmont, CO 80501

211. An Advanced Multisensing Coriolis Gas-Flow Meter

Cage, D.R.

This project is developing a new multisensing gas flow meter that can accurately measure the mass flow rate, pressure, density, temperature, and viscosity of any gas in a pipeline. All measurements are taken from a single

rugged nonintrusive and simple device that uses a unique method to create and utilize Coriolis forces to directly measure the mass flow rate of any gas moving in a pipeline. By virtue of an unusual sensor design and signal processing method, the same signals generated from the device to measure mass flow rate can also be used to concurrently measure gas pressure, density, temperature, and viscosity, all in real time with an estimated response of a fraction of a second. The Phase I research activities attempt to (1) fully understand this unique Coriolis effect, (2) gain the ability to predict the magnitude of the effect on any arbitrary sensor design, and (3) analyze the relationship between the effect and fundamental gas properties such as temperature, pressure, and density. The capability of this technology will then be compared with that from currently available alternative technologies.

Integrated Systems, Inc.
Santa Clara, CA 95054

212. Hidden Markov Modeling for Intelligent Control of Industrial Processes

Kosut, R.

The principal objective of Phase I is development of methods for obtaining process models from in situ and postmortem measurements that can be used for either quality control or feedback control. A novel feature of this approach is to identify the process by using the Hidden Markov Model (HMM), which has been used extensively in speech recognition. HMMs provide a natural means to use data for identifying a complex, uncertain, nonlinear system such as a processing plant. In Phase I, the HMM methodology is being extended for control system design, trained with simulated and actual data, and tested. A second related objective, more suited to Phase II, is development of computer-aided control engineering (CACE) design tools that appeal to the needs of process control engineers. Despite many theoretical and computational advances in the control sciences, there remains a substantial gap in its application by engineers in the process industries, where such a design approach could significantly enhance productivity. With the appropriate CACE tools, these engineers can perform sophisticated designs without demanding substantial increases in skill level. Such tools also extend the life cycle of control designs, decreasing the need for maintenance of control loops. The overall benefit to the process industries is improved performance from automation projects, which enables more profitable, cleaner, and safer operation of process plants.

IntelliSense Corporation
Boston, MA 02115

213. An Inexpensive Miniature Positioning Instrument for Intelligent Control Systems

Maseeh, F.

Significant commercial opportunities exist for systems that can control such industrial processes as those used for the intelligent control of a robot. This multiphase project addresses the development of a novel miniature, low-cost spatial tracking (positioning) instrument to be used in intelligent control systems. This instrument utilizes miniature sensors (microsensors) that are fabricated by using micromachining techniques. The objective of the Phase I work is to define the system specifications, including the requirements of the sensors, their interface electronics, and a microprocessor suitable to develop the instrument. During the subsequent phases of the program, the components defined during Phase I will be built, assembled, and tested. This includes developing a new solid-state angular rate sensor that meets the identified requirements. The developed positioning instrument will be commercialized through a collaborative joint venture approach. The self-contained instrument will be smaller and lighter than any available positioning instrument with similar characteristics. Its production cost could be several times less than those of similar systems.

Lektrox Company
New Port Richey, FL 34654

214. Improved Control of Pulp and Chip Refining through Direct Measurement of the Number and Severity of Fiber Impacts

Brenholdt, I.R.

The objectives of Phase I were (1) to construct a sensor incorporating new methods for measuring electrical impulses in the refiner housing; (2) to demonstrate the capability of the sensor to acquire and process the signal in a pilot-plant refiner on a single wood species; and (3) to show that the acquired signal correlates with traditional methods for measuring refining results, such as horsepower days per ton, pulp freeness, and the physical properties of hand sheets made from these pulps. These limited objectives have been met. It is well known in the industry that there are many process variables that influence a given pulps response to refining action. A major objective of Phase II is to learn how these variables influence the output of the new sensor, and to what extent this new measurement, derived from the refining action itself, predicts both drainage and paper properties for a wide range of typical mill conditions. These typical conditions will include other types of pulp (e.g., unbleached, hardwood, and recycled). The effects of pH, conductivity, and zeta potential will also be determined. These results will lead to the development of a control strategy that will be demonstrated in a mill site. Another important objective of Phase II will be to determine the capability of the sensor to measure and control chip refining.

On-Tech Joint Venture
East Hartford, CT 06138

215. A Rugged Stable Fourier Transform Interferometer for Process Monitoring

Solomon, P.

Innovative concepts are needed in advanced online sensors for application in industrial control systems leading to decreased energy consumption, better environmental

control, better quality control, and increased productivity in U.S. industry. During the last several years, Fourier Transform Infrared (FT-IR) spectroscopy has been identified as an important new tool to obtain species composition, concentrations, and temperature data in process monitoring. If FT-IR is to realize its potential in process monitoring, improvements must be made in mechanical stability, thermal stability, ruggedness, size, weight, cost, and serviceability of the instrument. This project addresses the development of an advanced process FT-IR based on innovative technology that will allow it to have the required properties for process monitoring. The technology is the subject of four patent applications. The Phase I tests are determining vibration tolerance, ruggedness, energy throughput, potential speed, and potential maximum resolution, among other properties. A prototype will be designed on the basis of these results.

Pen Kem, Inc.
Bedford Hills, NY 10507

216. Development of a Dielectric Spectroscopy

Goetz, P.

This project focuses on designing a stable and robust microsensor probe for dielectric spectroscopy that is capable of operating over a wide frequency range and eliminates all known problems in the measurement systems used at various laboratories. To interpret the dielectric spectra, deconvolution methods are being developed to estimate the particle-size distribution function and the surface-charge density. Finally, tests are being conducted on well-formulated and well-characterized colloidal suspensions to evaluate performance of the microsensor probe and deconvolution algorithms. The innovation results from a combination of (1) expertise in design of electrical signal processing for colloidal instruments involving microelectrophoresis and vibration potential to obtain particle zeta potential and (2) experience in deconvolution of ultrasound and Fourier Transform Infrared (FTIR) spectra to obtain particle-size distributions. Phase I of the project addresses the issues of designing a specialized microsensor probe for dielectric spectroscopy and developing deconvolution of dielectric spectra through inversion Fredholm integrals in complex number domain. This sensor is expected to meet the needs of industry in the field of size and charge characterization of colloidal systems with low-density contrast, where the ultrasound-based sensors currently available or under development are found to be of limited use.

Photonic Sensor Systems, Inc.
Atlanta, GA 30318

217. A Novel Integrated Optic Sensor for Inline Measurement of Mixing Quality in Chlorine Dioxide Pulp Bleaching

Chiang, H.K.

This project addresses the development of an inline sensor for measuring mixing quality in chlorine dioxide pulp bleaching. The sensor is based on a proprietary, integrated optical interferometer. The interferometer's unique design minimizes thermomechanical noise to provide a highly stable platform capable of detecting low concentrations of specific chemicals in fluid environments with high spatial resolution. The approach relies on the detection of small refractive index changes in a thin surface film. Specificity for chlorine dioxide is achieved by using a surface film that is reactive or interactive with chlorine dioxide. A mixing sensor based on this approach has several key advantages: (1) it allows real-time, continuous, in situ monitoring; (2) it has a broad dynamic range, yet is capable of sensitivities down to the parts-per-billion (ppb) level; (3) it can be fully reversible; and (4) it permits spatial resolution well below 1-mm. The resulting product will be suitable for assessing both macroscopic and microscopic mixing, and it will permit automated feedback control of pulp mixers. Moreover, development of sensors for other bleaching chemicals (e.g., ozone, hydrogen peroxide) would be a direct extension of this effort. In Phase I, a preliminary selection of candidate waveguide coatings will be made and they will be screened and optimized for their response to aqueous solutions of chlorine dioxide.

Research & Manufacturing Co., Inc.
Tucson, AZ 85714
Department of Thermosonics

218. Novel Ultrasonic Thermometers with Nonmetal Sensing Elements for Hostile Environments

Varela, D.W.

The objectives of this research project are to develop and test ultrasonic thermometers with nonmetal sensing elements for temperature measurement and control in highly corrosive manufacturing environments. Candidate nonmetal materials for the sensing element include sapphire, zirconium oxide, graphite, silicon carbide, and hafnium oxide. The Phase I research concentrates on the design, fabrication, and in-house furnace testing and calibration of ultrasonic sensors fabricated from these candidate materials. Phase II will be devoted to installing, evaluating, and qualifying the sensors (selected from the Phase I research) in production plants where the process is so corrosive that it precludes the successful use of conventional instruments. Nonmetal sensors can potentially eliminate sensor degradation from chemical and erosive attack, thus improving and, in some situations, making possible for the first time the real-time control of many industrial processes.

TPL, Inc.
Albuquerque, NM 87109

219. A Noninvasive Elemental Analysis System for Process Control in Harsh Environments

Tiernan, T.C.

Many industrial processes are not controlled in real time because they lack control sensors and systems suitable for use in extremely harsh environments. Neutron activation

analysis (NAA) is a noninvasive technique that exposes a sample to neutrons and examines the gamma rays emitted as a result of scattering and nuclear reactions. The gamma ray spectrum provides detailed information on the identity and quantity of the elements present in the sample. NAA has the potential to provide rapid, accurate, noninvasive elemental analysis in a variety of harsh industrial process control applications. Although NAA is currently used in areas such as oil well logging and scanning of airline luggage for explosives, its potential has not yet been fully realized, even in those fields, largely because of the performance limitations of existing radiation detectors. In particular, available detectors lack the combination of high speed, high stopping power, and good spectral response required for fast data collection; minimum pulse pileup and summing effects; and rapid, detailed elemental analysis. A novel scintillating material has recently been developed with the combination of high density and photoelectric cross section, ultrahigh speed, and scintillation efficiency required for real-time noninvasive process control based on NAA. This new technology is being developed for process control in harsh environments. In Phase I, scintillator material is being synthesized, fabricated into detectors, and evaluated.

INSTITUTION INDEX

This index lists the institutions responsible for the projects cited in this publication. The corporate names are entered in standardized forms found in the authority listing *International Energy Research Organizations* (ETDE/PUB-3). Each entry includes the project title and citation number.

INVESTIGATOR INDEX

Investigators' surnames are indexed in the form appearing in the citation; given names generally have been reduced to initials. For projects with multiple investigators, each name is indexed. Accent marks are not input because of computer alphabetization. Spelling and transliteration follow standard conventions.

SUBJECT INDEX

This index is arranged by subject descriptors selected from those assigned to each citation in this publication. Subject descriptors are selected from a controlled thesaurus of terms, *International Energy Subject Thesaurus* (ETDE/PUB-2). In order to enhance indexing, subject descriptor entries generally consist of a pair of descriptors: a main term and a qualifier term. Each entry includes the full title and the citation number.

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