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**THE CHEMICAL TECHNOLOGY DIVISION
AT ARGONNE NATIONAL LABORATORY:**

APPLYING CHEMICAL INNOVATION TO ENVIRONMENTAL PROBLEMS

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inside front cover

The Chemical Technology Division is one of the largest technical divisions at Argonne National Laboratory, a leading center for research and development related to energy and environmental issues. Since its inception in 1948, the Division has pioneered in developing separations processes for the nuclear industry. The current scope of activities includes R&D on methods for disposing of radioactive and hazardous wastes and on energy conversion processes with improved efficiencies, lower costs, and reduced environmental impact. Many of the technologies developed by CMT can be applied to solve manufacturing as well as environmental problems of industry.

Argonne National Laboratory is operated by the University of Chicago for the U.S. Department of Energy.

INTRODUCTION

"Many of our technology-related problems arise because of unforeseen consequences when apparently benign techniques are employed on a massive scale," says the historian of technology Melvin Kranzberg. These pressing

problems demand the best solutions science can offer. The scientists and engineers in the Chemical Technology Division (CMT) at Argonne National Laboratory draw upon their wide-ranging expertise to create innovative, cost-effective techniques for addressing the legacy of past and present governmental and industrial practices. These efforts have resulted in processes and devices for environmental control and restoration, including methods for treating many different types of hazardous waste, minimizing waste volume, and controlling and monitoring air pollution. These methods can be used in energy and other industries to support efforts to be good stewards of the nation's environment.

Many of CMT's programs are sponsored by the U.S. Department of Energy (DOE). The DOE is committed to increasing the exchange of ideas between the national laboratories and U.S. industries by transferring technologies from the laboratories and fostering collaboration through cooperative R&D agreements. A number of such agreements have already resulted from CMT activities. The largest of these involves the big three automakers (Chrysler Corp., Ford Motor Co., and General Motors) and the Electric Power Research Institute. The objective is to improve advanced batteries so that electric vehicles will be competitive with internal combustion vehicles. Other industrial collaborators include 3M Corp., Hydro-Quebec, SAFT America, Inc., NALCO Chemical Co., Amoco Corp., MC-Power, International Fuel Cells, and American Superconductor Corp.

The Division brings to these collaborations a unique collection of testing and analytical facilities, as well as a multidisciplinary research staff. The staff includes chemists, chemical engineers, materials scientists, geologists, mechanical engineers, and electrical engineers.

This booklet showcases selected technologies for which the Division has made significant advances. The Division stands ready to collaborate with industry in solving its environmental or manufacturing-related problems. For further information, call Dr. James Laidler, CMT Division Director, at 708-252-4479.

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APPLYING SEPARATIONS SCIENCE TO WASTE PROBLEMS

The chemicals to which life is asked to make its adjustment are no longer merely the calcium and silica and copper and all the rest of the minerals washed out of the rocks and carried in rivers to the sea; they are the synthetic creations of man's inventive mind, brewed in his laboratories, and having no counterparts in nature.

Rachel Carson, *Silent Spring* (1962)

Separation of Ultrafine Particles from Waste

The Chemical Technology Division, recognized worldwide for its expertise in separations science, specializes in developing innovative processes for treating contaminated soils, wastewater, solid nuclear wastes, and other liquid and solid waste. One such process involves grinding of solid waste to an average particle size of about one micrometer, followed by selective partitioning of the ultrafine particles between two immiscible aqueous phases. This aqueous biphasic separation process will recover most of the contaminants in a concentrate that has a volume of only a few percent of the initial waste volume. An application of this process being investigated involves recovery or concentration of refractory materials from incinerator ash, ash heels, and metallurgical processing residues. Also under investigation are removal and concentration of uranium from contaminated soils at the DOE Fernald site in Ohio and selective partitioning of radionuclides (TcO_4^- and I^-) from the caustic supernate in the high-level waste storage tanks at the DOE Hanford site.

Pilot plant developed for cleaning uranium-contaminated soil by aqueous biphasic separation

Schematic of aqueous biphasic separation for uranium-contaminated soil. This process partitions ultrafine uranium particles to an aqueous salt phase and the cleaned soil to a water-soluble polymer. The water-soluble polymers used in biphasic formation are inexpensive, nontoxic, and biodegradable.

Biocatalytic Destruction of Nitrate and Nitrite

Many of the aqueous wastes that have accumulated from DOE defense operations possess high nitrate and nitrite concentrations, which present a disposal problem. For example, if treated by high-temperature vitrification, these wastes will generate significant quantities of nitrogen oxides and can become chemically unstable and potentially explosive. The disposal problem would be minimized if the nitrate and nitrite in the waste were destroyed before preparation of the final waste form. We are thus developing a process that combines aqueous biphasic separation with immobilized enzymes for reducing nitrate and nitrite to innocuous products, namely, elemental nitrogen and water. Although this process is being developed for defense waste streams, it also has application to other nitrate-containing streams in the industrial sector, such as chemical plant discharge and drinking water.

Schematic of biocatalytic reactor for destroying nitrate (NO_3^-). The process combines immobilized enzyme technology with aqueous biphasic separation. A key part of the process is the partitioning of the nitrate into a polyethylene glycol (PEG) aqueous phase before enzymatic reduction. This allows the enzymes to be isolated from the harsh environment of the aqueous waste streams.

Centrifugal Contactor for Treating Liquid Radioactive Waste

We have developed an annular centrifugal contactor for use in liquid/liquid solvent extraction. Our primary goal has been to quickly and efficiently recover transuranic elements and fission products from liquid radioactive waste. The CMT-designed centrifugal contactor has several advantages over other solvent-extraction equipment currently in use. It requires less solvent, is easily modified to handle different solvent compositions, can be remotely operated and maintained, and has low construction and operating costs. Also, its high extraction efficiencies (above 99%) and low solvent holdup allow a pilot-scale unit to attain steady state with less than a liter of feed. Because of these advantages, the contactor has become the standard for performing solvent extraction in the DOE community. Units have been operated at Argonne, Westinghouse Hanford, Pacific Northwest Laboratory, Los Alamos National Laboratory, Westinghouse Idaho, Rocky Flats Plant, Y-12 Plant, Savannah River Site, and Oak Ridge National Laboratory. The benefits that make the centrifugal contactor the equipment of choice in the nuclear industry would be of value for waste treatment in the pharmaceutical, biotechnology, and metallurgical industries. In a related effort, a computer model has been developed to design flowsheets for implementing solvent extraction processes with centrifugal contactors as well as mixer settlers and pulsed columns.

Schematic of a single centrifugal contactor used for solvent extraction. The aqueous waste enters the contactor and is mixed with an organic solvent, which extracts the contaminant. The two liquids are then separated by centrifugal force inside the rotor. Multiple contactors are connected in series to run a flowsheet.

Electrometallurgical Treatment of Spent Nuclear Fuel

Researchers in the Division have developed a compact, efficient method for conditioning spent nuclear fuel for disposal. The method, known as "electrometallurgical treatment," separates fission products and transuranic elements from the larger quantity of uranium present in spent fuel. The pure uranium product can be stored, recycled, or converted to an oxide for disposal as a low-level waste. The fission products and transuranic elements are immobilized in highly stable waste forms. Compared with conventional reprocessing technologies, the electrometallurgical technology holds promise for significantly reduced costs, decreased volumes of high-level radioactive waste, and negligible volumes of secondary or low-level wastes. The method could facilitate the timely and environmentally sound processing of most of the nearly 3000 tons of spent nuclear fuel accumulated within the DOE complex.

The expertise in high-temperature thermodynamics, fluid handling, and containment materials resulting from the CMT's past work on electrometallurgical technology is applicable to numerous areas, both nuclear and non-nuclear. These areas include the extraction of plutonium from actinide-bearing waste that has been generated in defense programs, treatment of enrichment tailings from nuclear plants, and low-cost production of lanthanides useful to the metals industry.

Electrometallurgical process for treating spent nuclear fuel. Uranium from the dissolved fuel deposits on the solid cathode. Transuranics, active metal fission products (FPs), and rare earth FPs remain in the salt, from which they are extracted for immobilization. Noble metal FPs and some rare earth FPs are recovered in the anode basket.

Uranium deposited on cathode by electrometallurgical process

Waste Forms for the Electrometallurgical Treatment

Operations from the electrometallurgical treatment will result in two waste streams: a metal stream consisting of fission products and cladding hulls from the spent fuel, and a salt stream that contains fission products and transuranics. We have developed processes for treating and packaging these waste streams. The metal waste stream is handled by a melting step that removes the transuranic elements and produces a high-level waste form. The salt waste stream is passed through a zeolite bed that absorbs the transuranics and fission products. The zeolite loaded with fission products is hot pressed with a glass frit to produce a second high-level waste form. Both the mineral waste form and the metal waste form are stable under envisioned repository conditions and are highly resistant to leaching of waste elements. Large glovebox facilities have been built in CMT for carrying out experiments with zeolite and metal waste forms, as well as other radioactive materials and processes that must take place in a protected atmosphere.

The technology resulting from this work could also be applied to waste streams from production of special nuclear materials, nonradioactive toxic wastes such as barium-contaminated salts from industrial processes, and industrial wastes bearing contaminants such as heavy metals.

Extensive glovebox facilities built in CMT for conducting experiments with radioactive wastes

Glassy Waste Forms for Radioactive and Hazardous Waste

Glasses are the primary candidate waste form for disposing radioactive waste intended for a geologic repository. The CMT Division has over 15 years experience in preparing glass forms containing nuclear waste materials and evaluating their performance under simulated repository conditions. This expertise is now being applied to the vitrification of DOE wastes with relatively low levels of radioactive and hazardous elements. A new vitrification method, developed in CMT, blends several waste streams to minimize the amounts of glass-forming additives necessary and thereby reduce costs. This method produces a stable glass waste form of minimum volume. A similar method is also being explored for producing a glass-crystalline composite for handling waste streams that are difficult to vitrify. Product durability is evaluated by using test methods developed for high-level nuclear waste and adapted for use with other kinds of waste.

This vitrification method is also applicable to commercial toxic and nontoxic wastes. For example, it could convert industrial spent catalysts into valuable products, such as glass frits, abrasives, and architectural products.

Simulation of the reaction of nuclear waste glass with water. As the glass reacts, actinides (blue areas) release to solution as colloidal particles. Used in modeling of nuclear waste repository integrity.

Ion Replacement Electrorefining of Metals and Molten Salts

We have invented several new metal separation and purification processes as a result of past work on treating spent reactor fuel. One such process, called ion replacement electrorefining, overcomes the shortcomings of conventional electrorefining and electrowinning and could lead to improved processing capabilities for purifying a variety of metals and recovering oxidized metals from molten salts. It uses liquid sodium contained in a β -alumina tube as a cathode during metal dissolution in a molten salt electrolyte, then as an anode during metal separation and deposition on inert cathodes. One application of this process is separating transuranic elements from fission products that occur in typical radioactive waste forms generated by commercial nuclear reactors and by the defense nuclear programs. The beta-alumina/sodium electrode also has potential as a reliable reference electrode for use in molten salts. Such an electrode, when combined with electroanalytical methods such as potentiometric and voltammetric analysis, could yield better sensors for monitoring and controlling industrial high-temperature processes.

Schematic of ion replacement electrorefining for purifying metals. The metal to be purified is first dissolved in a molten salt, then deposited in pure form on an inert cathode.

DEVELOPING POWER SOURCES WITH MINIMAL ENVIRONMENTAL IMPACT

The true history of the United States is the history of transportation.

Winston Churchill (1942)

The scientist describes what is: the engineer creates what never was.

Theodor von Kármán (1980)

High-Performance Batteries for Electric Vehicles

Several states already require auto manufacturers to make "zero emission" vehicles (such as vehicles powered by batteries or fuel cells) available for sale, and other states are considering such requirements. Electric vehicles require batteries that are affordable, meet or exceed current safety standards, and meet customer expectations for performance. We are developing a bipolar lithium/sulfide battery that shows great promise for meeting all these requirements. This battery employs disk-shaped voltaic cells assembled into a series-connected stack in which adjacent cells share a common current collector, called the bipolar plate. Each cell contains lithium-alloy anodes, iron sulfide cathodes, magnesium oxide separators, and a molten salt electrolyte. A key breakthrough was developing sulfide ceramics that form ceramic-to-metal seals which remain strong under highly corrosive conditions. Compared with present-day technology, this new battery could provide up to five times as much energy and operate ten times longer.

The Division is also developing lithium-polymer batteries, which show considerable potential for meeting the demanding performance requirements of electric vehicles and operate at low temperature (below 100°C). They are assembled from lithium-polymer sandwiches that are extremely thin, sometimes less than a few thousandth of an inch. The battery's flexible, multilaminate structure makes possible very high power and energy densities. The use of a solid polymer as the electrolyte is particularly advantageous because it does not leak, corrode components, or emit dangerous gases.

Exploded view of bipolar lithium/sulfide battery stack designed for application in electric vehicles

First lithium-polymer cell developed in collaborative effort involving CMT, Hydro-Quebec, and 3M Corp.

Battery Analysis and Diagnostic Laboratory

Since 1976, researchers have used CMT's Battery Analysis and Diagnostic Laboratory to test battery systems for applications such as zero emission vehicles and utility load-leveling during peak demand periods. The facility houses two laboratories: a computer-operated test laboratory and a post-test analysis laboratory. In the test laboratory, individual cells and multicell modules of battery systems are subjected to performance and lifetime tests under simulated real-world conditions. In the post-test laboratory, researchers subject failed cells (in a protected atmosphere, if needed) to analyses to assess component reliability and correlate operational performance with material changes. To date, the Analysis and Diagnostic Laboratory has tested over 3000 cells, configured into multi-cell modules and full-size batteries. These units represent 13 types of battery systems provided by 18 battery developers.

This facility provides a place where researchers can apply unbiased tests and analyses, thereby establishing a common basis for evaluating battery performance and life. The information from these evaluations allows battery developers and program managers to measure technical progress and identify areas in which changes in the design or in construction materials might improve battery performance.

High-performance batteries in Analysis and Diagnostic Laboratory being tested under simulated application conditions

Advanced Fuel Cells for Transportation

Research is underway to develop fuel cells for zero and ultra-low emission vehicles. Besides being nonpolluting, fuel cells operate quietly and contain no moving parts. Such fuel cells could replace the internal combustion engine in a wide array of transportation applications, including cars, trucks, buses, trains, and ships.

Because of their low operating temperatures (80°C), the polymer-electrolyte fuel cells are targeted for transportation applications. For a zero emission vehicle with this fuel cell, hydrogen must be carried on board. Hydrogen may also be produced by on-board reforming of fuels such as natural gas or alcohols. However, the fuel reforming process leads to a hydrogen-rich gas mixture containing substantial quantities of carbon dioxide and some carbon monoxide. The latter, in particular, decreases the efficiency of the platinum anode catalyst and lowers the power generated by the polymer-electrolyte fuel cell. We are applying sophisticated experimental and analytical techniques to explore economical electrocatalysts that are not susceptible to poisoning by carbon monoxide. In a related activity, we are developing an advanced fuel reformer that offers rapid startup and excellent performance, and is expected to be compact, lightweight, and low cost.

Together with Georgetown University, the CMT Division manages efforts by industrial contractors in the Fuel Cell Bus Project. The contractors are building a small fleet of urban transit buses powered by phosphoric acid fuel cells combined with batteries, where the fuel cell provides the total energy needed while the battery provides the short-duration power needed during bus acceleration and absorbs the energy of regenerative braking.

Fuel reformer developed for converting alcohols to hydrogen for use in vehicles powered by fuel cells

Urban transit bus powered by advanced fuel cell. Developed as part of university-industry-Argonne collaborative effort.

Advanced Fuel Cells for Utilities

Fuel cells can convert the chemical energy of nonpetroleum fuels such as hydrogen, methanol, or ethanol to electricity with little or no pollution and with greater efficiency than heat engines. We are conducting R&D on a solid oxide fuel cell and a molten carbonate fuel cell, both of which are targeted for use as small power plants in utility applications such as hospitals.

For the solid oxide fuel cell, we are developing new electrodes, electrolytes, interconnect materials, and processing techniques to reduce the operating temperature from the present 1000°C to 800°C, or even lower. At these lower temperatures, manufacturing costs would be reduced, operating efficiency increased, and cell durability improved. We have also developed glass and glass/ceramic materials to seal along the edges of each cell and between the gas supply manifold and fuel cell stack. These sealants are able to seal different cell components and withstand the requisite cell operating temperatures and gas compositions.

In the present molten carbonate fuel cells, the nickel oxide cathodes limit cell lifetime because of dissolution and migration to the nickel anode. We have developed lithium ferrate and lithium cobaltate cathodes that are expected to yield the long cell lifetimes (over 40,000 hours) needed for utility applications. In addition, advanced cell designs are being developed for higher power density and lower cost. The power density is being increased through the use of multiple gas manifolding, pressurized operation, and design optimization. The cost is being reduced through eliminating complex and expensive stamped metal parts that currently form the gas flow channels, the electrode supports, and the current collectors for each cell.

Flow visualization of anode and cathode gases in molten carbonate fuel cell. Done by injection of NH_3 -saturated air imaged on Oزالid paper and used in design optimization.

FINDING CREATIVE SOLUTIONS TO AIR-BORNE POLLUTION

The battle for a sustainable environment will be won or lost in the urban centers of the developing world. We've got to operate as if we believe we can solve these problems.

Maurice Strong, *Washington Post* (1994)

Made-to-Order Catalysts for Treating Engine Exhaust

We have discovered an innovative method for creating diverse, novel materials for catalysts, which can be tailored for specific applications. These new catalysts have the potential to remove far greater quantities of nitrogen oxides, unburned hydrocarbons, and other pollutants than do current catalysts. These catalysts are created by a special synthesis that involves modifying molecular sieve materials (like zeolite-Y) with large pore sizes. With this method, we have produced materials containing catalytically active molecular clusters. A variety of cluster types can be created by simply changing the pore size of the molecular sieve or making suitable adjustments to the encapsulated cluster. Transition metal sulfide, nitride, and carbide clusters have been synthesized in the pores of several molecular sieves.

The possible applications of these new catalysts are diverse. For example, they can be used in automobile catalytic converters for treating engine exhaust. They have also been investigated as a means to develop more efficient processes for producing motor fuels from natural gas.

Catalyst formed from molybdenum/sulfur clusters encapsulated in the supercages of Type-Y zeolite

Incineration without Direct Emissions

A conceptual design has been developed for a closed-loop process that will prevent the accidental release of toxic gases during incineration of hazardous and mixed radioactive wastes. With conventional off-gas treatment systems, it is not possible to instantaneously detect and prevent accidental releases created by process upsets, equipment malfunctions, or operational errors. Also, hazardous materials tend to concentrate on ultrafine particles, which are difficult to collect and can be released to the environment. Unlike conventional systems, the off-gas treatment process designed in CMT has no direct gaseous emissions to the environment. The process can safely treat combustion products from all types of commercially available incineration and vitrification systems, and it can be retrofitted to existing facilities so that they are more acceptable to the public and regulatory authorities.

Schematic of closed-loop system designed for preventing release of toxic materials after waste incineration. Instead of being sent up the stack, the combustion gas is filtered to remove particulates and sent to a condenser to remove water. About 80% of the relatively dry stream is recycled back to the incinerator with added oxygen, and 20% is diverted to a side loop to remove CO₂ and contaminants that build up after several combustion cycles.

Continuous Emission Monitor for Organic Pollutants

Many industrial processes require devices to monitor chemicals released into the environment via stack releases or other routine industrial emissions. We have developed a continuous emission monitor that may be the first such instrument accepted by the U.S. Environmental Protection Agency for measuring emissions from thermal processors as an aid in pollution control. This monitor combines specially designed computer software with an analytical instrument (based on Fourier transform infrared spectroscopy) into a unit that can detect the presence of numerous chemicals at one time. The monitor can identify organic pollutants that are hard to find because they are present in very small amounts (parts per million level) or difficult to detect by other methods. Using analytical data from this instrument, operators of thermal processors could make appropriate adjustments in operating conditions to ensure clean and complete burning. The monitoring technology can be applied to emissions from vitrification facilities, arc melters, incinerators, and stacks from other types of thermal treatment facilities. In a related program, we are also investigating the use of Fourier transform infrared technology for detecting chemicals from remote locations.

Monitoring of stack gas emissions with CMT-designed instrument.

Portable Analyzer for Atmospheric Pollutants

An infrared aerosol analyzer has been developed to identify and quantify atmospheric pollutants that contribute to acid rain and other health concerns, such as the respiratory problems of asthma patients and the elderly. This portable instrument collects size-fractionated samples of aerosol particles from the ambient atmosphere particles and analyzes them with Fourier transform infrared spectrophotometry. It provides broad-range analysis in real time with no sample handling or preparation, unlike other instruments that are limited to a specific detection task and require lengthy periods for sample collection and analysis. The infrared spectra produced by this instrument yield characteristic fingerprints for a wide variety of organic and inorganic chemical matter, including hydrocarbons, petrochemicals, nitrates, sulfates, and many toxic and hazardous materials.

Infrared aerosol analyzer for atmospheric pollutants that cause environmental problems such as acid rain

APAPTING ADVANCED TECHNIQUES AND MATERIALS TO INDUSTRIAL NEEDS

Does the mason want a cement? Does the dyer want the means of tinging a cloth of a particular colour? Or does the bleacher want the means of discharging all colours? It is the chemical philosopher who must supply these...Wherever any art requires a matter imbued with any peculiar physical properties, it is the chemical philosophy which either informs us of natural bodies possessed of these properties or induces such in bodies which had them not before, or lastly, produces new bodies imbued with the necessary qualities.

William Cullen (c. 1776)

Smart Chemical Sensors

The ultimate goal of environmental monitoring is "instantaneous" detection of target analytes. A CMT analytical chemist is designing unique data analysis algorithms for creating "smart" chemical sensors. The term "smart" means that sensors employing these algorithms would be capable of automated data analysis and decision making. These algorithms encode into a numerical procedure the visual and logical procedures that an expert uses to analyze sensor data. It does not matter whether the target analyte is a toxic gas or an impurity in a process stream, nor does it matter whether the detection is accomplished by spectroscopic, chromatographic, electrochemical, or radiochemical methods. Because the algorithms reduce analysis time and analytical costs and can be implemented as part of computer software or hardware, they have tremendous potential in such areas as on-line process control, on-site monitoring, and remote sensing. The resulting smart sensors provide important advantages in multisensor data fusion, in which multiple chemical sensors are connected to a central processing system.

ALIX15

Schematic for creating smart chemical sensors. Digital filters extract analyte information from background noise and interferences in raw signal. Pattern recognition procedures make an automated qualitative decision regarding the presence or absence of target analyte. Chemometric methods analyze the filtered data to obtain quantitative data.

High-Resolution NMR Probe for Material Structures

We have developed a relatively inexpensive technique that uses nuclear magnetic resonance (NMR) to probe the structures of ceramics, alloys, composites, and coatings. The new technique, "toroid cavity imaging," provides resolutions up to 100 times better than conventional MRI techniques. This technique was originally developed for high-pressure NMR studies, especially catalytic reactions that occur at high pressures, but has application in any research area where NMR spectral information is desired as a function of distance. For example, the probe is being used to map electrochemical events emanating radially, within a thin diffusion layer, from an electrode of a high-performance battery designed for an electric vehicle.

Toroid cavity detector developed for NMR investigations at high temperatures and pressures

Catalytic Processes for Generating Industrial Chemicals

Advances in basic chemistry research in CMT have led to the discovery of new catalytic processes for converting petroleum-based hydrocarbon feedstocks into alcohols and aldehydes that can be used as industrial solvents (for example, plasticizers), detergents, and agricultural chemicals. This research centers on modifying the commercial oxo processes used for the hydroformylation of olefins, a family of hydrocarbons. The modifications replace conventional separation of the catalytic products by distillation steps with more energy-efficient separations that use CO₂ in a supercritical fluid. They also make the oxo processes more environmentally benign by achieving cleaner separations and by replacing liquid solvents with relatively nontoxic, nonflammable, and easily recycled CO₂ gas. If the modified processes are successful, the overall benefits could be large, because the total U.S. hydroformylation capacity exceeds 5 million tons of product per year.

Concentrations of catalytic intermediates formed during the hydroformylation of propylene in supercritical CO_2 at 80°C and high pressure. These data were derived from *in situ* NMR spectra (inset) of reacting gas stream over time and are used in studies to improve catalytic processes.

New Quantum Chemical Method

In collaboration with researchers from AT&T Bell Laboratories and Carnegie Mellon University, a CMT theoretical chemist has developed a new quantum chemical method for calculating the total energies of compounds composed of light elements (atomic numbers 1 through 18). This powerful method, called the Gaussian-2 (G2) quantum chemical code, has led to improved calculated values (within 2 kcal/mole of observed data) for atomization energies, ionization energies, proton affinities, and electron affinities. The G2 code is now being widely used in universities and industry for the accurate calculation of thermochemical data. It offers tremendous possibilities for identifying new processes and novel materials without the need for exhaustive, unguided laboratory research and has relevance to applications in high-temperature industrial processes, catalysis, chemical synthesis, and assessments of chemical hazards or safety.

Calculated changes in potential energy for reaction of C_2H_5^+ with hydrogen. These G2 calculations are being used in a basic science study of zeolites (microporous crystals of enormous importance to the chemical industry).

High-Temperature Superconducting Materials

Argonne is a leader in developing a new class of materials called "high-temperature superconductors." These materials are attractive because they lose all electrical resistance when cooled to the temperature of liquid nitrogen (77 degrees above absolute zero). Working with an industrial partner (American Superconductor Corp.), we are developing a method for manufacturing long, durable lengths of superconducting wire made from a composite ceramic material: silver-sheathed $(\text{Bi,Pb})_2\text{Sr}_2\text{Ca}_2\text{Cu}_3\text{O}_x$. Both thermodynamic and microstructural methods are applied to investigate the phase evolution and microstructure development that take place during composite processing. This high-temperature superconducting product could be used in high-efficiency motors and generators, magnets, energy-storage devices, flywheels with low energy loss, fault-current limiters, and power-transmission lines.

Testing of silver-sheathed wire prepared with high-temperature superconducting materials

Mineral-Fluid Interactions in Systems Related to Natural Resources

We have been applying synchrotron radiation techniques to experimental studies of chemical processes occurring at mineral-fluid interfaces. Such processes control geochemical transport, including contaminant migration in groundwater aquifers, and are therefore of practical importance. For this work, we have developed and fabricated an X-ray transparent reaction cell. This novel device continuously monitors reaction progress as a mineral surface reacts with a fluid. Use of this cell, combined with other sophisticated analytical techniques, is applicable to a wide range of geochemical studies, such as contaminant transport in surface water and groundwater, nutrient cycling in agricultural systems, and compatibility of various industrial byproducts with the natural environment.

Crystal structure of calcite showing rhombohedral cleavage surfaces. Such crystals are used in geochemical studies of atomic-scale processes at the interface between rock (calcite) and water. Analyses of this interface are done with synchrotron X-ray techniques.

Materials Analyses with Brilliant X-rays

When completed in 1996, Argonne's Advanced Photon Source will generate the world's most brilliant synchrotron X-rays for materials research in a variety of fields. The CMT Division is part of a collaborative access team investigating possible synchrotron research activities suitable for the Advanced Photon Source. Team members include representatives from Amoco Corp., Notre Dame University, Northwestern University, Illinois Institute of Technology, and the University of Florida. A prominent goal is to develop capabilities to analyze environmentally relevant samples at a microscopic level never before possible.