Chemical Engineering Division

The Chemical Engineering Division is a diverse early-stage engineering organization specializing in the treatment of spent nuclear fuel, development of advanced electrochemical power sources, and management of both high- and low-level nuclear wastes. Additionally, the Division operates the Analytical Chemistry Laboratory, which provides a broad range of analytical services to Argonne and other organizations, and the Electrochemical Analysis and Diagnostics Laboratory, which provides independent, standardized battery and fuel cell testing and analysis.

Currently, we are engaged in the development of several technologies of national importance, including

- Aqueous and pyrochemical processes for the disposition of spent nuclear fuel,
- Stable nuclear waste forms suitable for storage in a geological repository,
- Fuel cells and hydrogen production and storage for polymer electrolyte and solid oxide fuel cell systems, and
- Advanced lithium-ion and lithium-polymer batteries for transportation and other applications.

Our basic science programs are engaged in research projects such as catalysis and superconductivity that have the potential to impact future energy systems. The Division also serves as a source of technical support for national security, radiochemical analysis and characterization, and other areas requiring specialized expertise.

Nuclear Technology

The Chemical Engineering Division is a leader in pyrochemical process research and development. The emphasis of our recent work has been on closing the nuclear fuel cycle, which consists of the treatment of spent nuclear fuel to recover actinides for use in advanced reactor systems and to encapsulate fission products in durable waste forms for storage in a geologic repository.

Throughout process development activities, our focus has centered on the development of commercially viable technologies—technologies that produce a high-quality product, can be scaled up, integrate seamlessly with other fuel processing steps and facilities, and are economic.

- Pyrochemical process development and demonstration to enable nuclear fuel cycle closure
- Materials development and evaluation
- Transuranic element recovery from spent nuclear fuel for recycle into advanced reactor systems
- Conversion of metal oxides to base metals for subsequent treatment by electrorefining
- Evaluation and preliminary design of advanced pyrochemical process equipment concepts for use in a spent fuel treatment facility

Contact Mark Williamson, Head, Nuclear Technology Department (630-252-9627, williamson@cmt.anl.gov)

There is a growing consensus in the United States and abroad that a significant growth in nuclear energy must occur and that it must be accompanied by the development of advanced fuel cycles that are proliferation-resistant, sustainable, and decrease the amount and long-term hazards of nuclear waste.
This policy direction is reflected in the National Energy Policy, approved by the President in May 2001, which addressses the continued development of an advanced nuclear fuel recycling technology commonly known as pyroprocessing. The Policy specifically states:

. . . United States should reexamine its policies to allow for research, development and deployment of fuel conditioning methods (such as pyroprocessing) that reduce nuclear waste streams and enhance proliferation resistance. In doing so, the United States will continue to discourage accumulation of separated plutonium, worldwide.

The United States should also consider technologies (in collaboration with international partners with highly developed fuel cycles and a record of close cooperation) to develop reprocessing and fuel treatment technologies that are cleaner, more efficient, less waste intensive, and more proliferation resistant.

The National Energy Policy Group goes on to recommend the development of advanced nuclear systems to meet the United States' projected energy needs over the next several decades, including the growing demand for electricity and production of alternative fuels such as hydrogen.

The U.S. Department of Energy, through its integrated Generation IV (Gen IV) and Advanced Fuel Cycle Initiative (AFCI) programs, will develop and demonstrate the next generation of advanced nuclear systems, to meet future needs for safe, economic, sustainable, proliferation-resistant and environmentally responsible fuel cycles and energy production.

Process Chemistry and Engineering

The Process Chemistry and Engineering Department conducts research that supports closing the nuclear fuel cycle and eliminating the use of highly enriched uranium in civil research programs throughout the world, and nanoscale engineering for biomedical and national security applications.

Under the Department of Energy's (DOE's) Advanced Fuel Cycle Initiative, Argonne is leading development of the UREX+ aqueous separations, a multi-step process for separating out the high-risk elements of spent nuclear fuel. Argonne has successfully demonstrated the entire process in hot cells and glove boxes and is preparing for scale-up demonstration.
We also provide support to DOE for its Yucca Mountain license application to develop and refine computer models that DOE can use to assess the repository's long-term performance.

- Develop processes and equipment for safe and economic treatment of nuclear waste
- Characterize leaching/degradation mechanisms for nuclear waste forms in the environment
- Develop a scientific basis for assessing waste form performance in the respository
- Develop waste form acceptance criteria
- Develop the means to convert molybdenum-99 production from high- to low-enriched uranium
- Develop industrial separations processes

Contact Monica Regalbuto, Head, Process Chemistry and Engineering Department (630-252-1540, regalbuto@cmt.anl.gov)

The mission of DOE's Reduced Enrichment for Research and Test Reactors (RERTR) is to develop the technologies necessary to convert research and test reactors from the use of fuels and targets containing highly-enriched uranium to the use of fuels and targets containing low enriched uranium (We support the RERTR Program at Argonne by developing new processes that allow the production of molybdenum-99 (the most commonly used medical isotope in the world) from low-enriched uranium targets. The Division's Remote Handling Mock-up Facility is a valuable tool in our research, allowing us to carry out and refine planned handling of radioactive isotopes in preparation for hot-cell experiments, saving considerable time and expense.

Advanced Lithium Batteries

DOE is helping industrial developers of high-power lithium-ion batteries understand the mechanisms that limit battery life and abuse tolerance. Efforts focus on identifying and developing advanced materials and cell chemistries that overcome these limitations, while reducing cell material and packaging costs. We also conduct longer-range research on novel materials to enhance the performance, life, and/or safety of advanced lithium batteries, while reducing cost. Recently we discovered new families of intermetallic negative electrode materials and layered metal oxide positive

Transportation (Hybrid/Fuel-Cell Electric Vehicles)
- Understand life and safety limiting mechanisms
- Develop novel materials and advanced cell chemistries to enhance power, life, and safety, while reducing cost
- Develop innovative approaches for reducing battery cell packaging costs

Specialty Applications
- Develop long-life cell chemistries for biomedical battery applications
- Develop high-energy cell chemistries for military and space battery applications

Contact Gary Henriksen, Head, Battery Department (630-252-4591, henriksen@cmt.anl.gov) electrode materials. Many of these materials are well suited for use in other rechargeable battery use such as consumer electronics, biomedical and space applications, and portable power sources for military use.

Battery and Fuel Cell Testing and Analysis

The Division operates the Electrochemical Analysis and Diagnostics Laboratory, which was established by DOE to conduct independent evaluations of advanced battery and fuel cell systems. Since it was established more than two decades ago, the laboratory has tested more than 4,000 cells and batteries, ranging from individual 4-Wh cells to 50-kWh batteries, representing numerous technologies and battery developers. The facility tests and evaluates fuel cell stacks and fuel cell systems up to 50 kW. Contact Ira Bloom (630-252-4516, bloom@cmt.anl.gov, www.cmt.anl.gov/facilities/eadl.shtml).

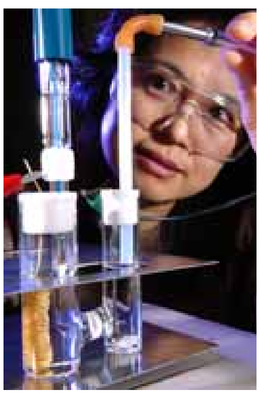
Hydrogen and Fuel Cells

Fuel cells offer a clean, efficient power source for transportation, as well as for residential and distributed stationary power generation. Argonne is working closely with the U.S. Department of Energy to help develop fuel cell materials, processes, and systems, as well as hydrogen production and storage materials for these uses.

Hydrogen is considered the ideal energy carrier for fuel cells in the long term but until hydrogen is readily available, fuel cells will need to use conventional fuels, such as natural gas, propane, gasoline, and diesel, or alternative fuels, such as methanol, ethanol, and bio-diesel. Such fuels can be converted to hydrogen or a hydrogen-containing gas mixture through a series of chemical reactions in "fuel reformers" (also known as fuel processors).

- Materials and systems for hydrogen production and storage for fuel cell systems
- Improved catalysts, processes, and reactor designs for fuel processing in integrated fuel cell power systems
- Improved, lower-cost, durable materials for fuel cells

Contact Romesh Kumar, Head, Fuel Cell Department (630-252-4342, kumar@cmt.anl.gov)



Fuel cell research at Argonne focuses on developing

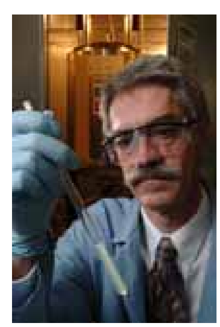
- Catalysts, processes, and reactor designs for fuel processing in integrated fuel cell power systems,
- Improved, lower-cost materials for fuel cells, and
- Materials for hydrogen production and storage for polymer electrolyte and solid oxide fuel cell systems.

One use for solid oxide fuel cells is auxiliary power units (APUs) for heavy-duty vehicles. A fuel cell APU would generate power for air conditioners and other hotel loads when the main engine is shut off, enabling truck owners to meet impending anti-idling legislation while improving their overall fuel economy. Argonne is developing a rugged solid oxide fuel cell, the TuffCell, that could be used for this purpose.

Argonne is also developing technology to reform diesel fuel for use in fuel cell applications. Thus, tractor-trailer trucks could soon be using diesel fuel not only for power to roll down the highway, but to create the hydrogen needed for clean, quiet, fuel-cell-powered APUs as well as for emissions control.

We are collaborating with three university teams to address materials and fuel processing issues.

Basic and Applied Research



The Chemical Engineering Division conducts research on fundamental issues involving chemistry and materials functionality in systems that are relevant to electric power distribution, energy efficiency enhancement, chemical manufacturing, and clean air technologies. Our investigations of high-temperature superconducting (HTS) ceramics for electric power emphasize the optimization of processing conditions for the Ag/Bi-2223 composite superconductor and the characterization of HTS-coated conductor embodiments employing biaxially textured $Y_1Ba_2Cu_3O_7$.

- Processing and characterization of ceramic oxides with high superconducting critical temperatures
- Heterogeneous and homogeneous catalysis
- Ion transport mechanisms in operating electrochemical devices and during corrosion

Contact Theodore (Ted) Krause, Head, Basic and Applied Research Department (630-252-4356, krause@cmt.anl.gov)

Research on homogeneous catalysis explores the effects of elevated pressure and solvent polarity on reaction kinetics for important industrial processes, e.g., the hydroformylation of olefins. Nanoscience methodologies are combined with multiphase media approaches and surfactant technology to develop new classes of catalysts exhibiting the combined beneficial characteristics of homogeneously and heterogeneously induced chemical reactivity. Focus areas in heterogeneous catalysis include the development of catalysts for reduction of NO_x emissions, advanced catalytic membrane reactors, and catalysis in relation to hydrogen production.

Our research on ion transport mechanisms focuses on issues of ionic mobility in battery systems for high power applications. The nuclear magnetic resonance-based imaging techniques developed in this program find broad utility as tools for in situ interrogations of the spatial disposition/distribution of chemically active species, defect structures in materials, and corrosion.

National Security

Within our nuclear forensics and nanoscale engineering group, tiny engineered spheres (smaller than red blood cells) are the key to revolutionary technology that could help detoxify humans following exposure to biological, chemical or radiological weapons. This technology could also provide better-targeted drug delivery (for example, help stroke victims by decreasing the side effects of invasive treatment and increasing the time window for successful treatment), provide earlier diagnosis, and selectively remove natural toxins that result from trauma or auto-immune disease (for example, cardiac arrest and lupus, respectively). We are working with six universities and a school of medicine. The group also is developing a system to safely capture and dispose of radioactive elements in porous structures outdoors, such as buildings and monuments, using a spray-on, super-absorbent gel and engineered nanoparticles. Contact David Chamberlain (630-252-7699, chamberlain@cmt.anl.gov).

The Analytical Chemistry Laboratory (ACL) has a full range of analytical capabilities for inorganic, organic, and radiochemical analyses and R&D. We have been involved in developing methods to determine chemical agents for the U.S. military and the EPA; developing methods for determining lithium, aluminum, and impurities in lithium aluminate for the Tritium Target Project; and producing laboratory-evaluation samples for the Waste Isolation Pilot Plant Head Space Gas Performance Demonstration Program. Using hot-cell and glovebox facilities, ACL analysts recently measured actinide and fission-product nuclides in very high burnup (64 GWd/tU) spent nuclear fuel from a light water reactor. The fuel burnup calculated from these data provided a benchmark value for comparison with the burnup predicted by computer code. Work is underway to extend the methods to include many more nuclides, particularly those of interest for benchmarking the high-burnup performance of computer codes that predict the time-dependent nuclide inventory and provide data needed for evaluating safety and licensing issues related to burnup credit. Contact Vivian Sullivan, Manager, ACL (630-252-1890, sullivan@cmt.anl.gov).

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