Separations and Analysis

Portfolio Description

This activity supports fundamental research covering a broad spectrum of separation concepts, including membrane processes, extraction under both standard and supercritical conditions, adsorption, chromatography, photodissociation, and complexation. Also supported is work to improve the sensitivity, reliability, and productivity of analytical determinations and to develop new approaches to analysis in complex, heterogeneous environments, including techniques that combine chemical selectivity and spatial resolution to achieve chemical imaging. This activity is the nation's most significant long-term investment in the fundamental science underpinning actinide separations and mass spectrometry. The overall goal is to obtain a thorough understanding, at molecular and nanoscale dimensions, of the basic chemical and physical principles involved in separations systems and analytical tools so that their full utility can be realized. Capital equipment funding is provided for items such as lasers for use in sample ionization and chemical imaging, advanced mass spectrometers with nanoprobes, confocal microscopes for sub-diffraction limit resolution, and computational resources.

Unique Aspects

This activity represents the Nation's most significant long-term investment in solvent extraction, ion exchange, and mass spectrometry. The supported research is characterized by a unique emphasis on underlying chemical and physical principles, as opposed to the development of methods and processes for specific applications.

Relationship to Other Programs

The activity is closely coupled to the Department's stewardship responsibility for actinide and fission product chemistry and to its clean-up mission. It emphasizes the separation and analysis of actinide and fission product elements and their decay products and is therefore naturally coordinated with the BES Heavy Element Chemistry Program. Similarly, elements of the analysis science portfolio benefit from cooperation with the BES Catalysis Science, Chemical Physics, Materials Chemistry, and Atomic, Molecular, and Optical Science Programs. The basic nature of the research has led to advances in technologies ranging from those that support nuclear non-proliferation efforts to those connected with advanced nuclear energy systems.

Significant Accomplishments

This activity is responsible for such recent notable contributions as the concept of host-guest complexation, which was recognized with the 1987 Nobel Prize in Chemistry; the use of the inductively coupled plasma (ICP) for emission and mass spectrometry; the development of the TRUEX process based upon fundamental research on ligand design; the development of SIMION, a program to simulate the motion of ions in fields, that has become the standard tool internationally for development of ion lens; and, more recently, the development of a new calixerene ligand that complexes Cs^+ that is based on design and development work performed by BES researchers at Oak Ridge National Laboratory (ORNL) and that is being used to clean up waste tanks at Savannah River National Laboratory (SRNL). The success of the Manhattan Project was, in large part, due to our ability to develop industrial-scale processes for separating plutonium from irradiated fuel. Thus began the intense interest of the Department of Energy and its predecessor agencies in the science that underlies separation processes. The missions of the Department have evolved, and it must now face the legacy of accumulated wastes from the cold war era and the growing emphasis on alternative energy sources. Knowledge of molecular-level processes is required to characterize and treat the extremely complex mixtures associated with cleanup and to predict the fate of associated contaminants in the environment.

Likewise, the Department and its predecessors were also driven to develop analytical methodologies to support their early missions. Nuclear and radiochemical analyses were supported and refined by developments in analytical separations, such as solvent extraction and ion exchange. A need for reliable potentiometric titration prompted the first use of operational amplifiers in analytical chemistry and led to a revolution in electrochemistry. Mass separation was required for assay in the form of mass spectrometry and, in the form of the calutron, served as the first method for the production of macroscopic quantities of separated isotopes of uranium and other elements. As with separation science, improved understanding of the underlying science is required to meet the analytical challenges presented by the legacy of the cold war, alternative energy sources, and the future challenges of the Department as its missions and responsibilities continue to evolve.

Mission Relevance

Work is closely coupled to DOE's stewardship responsibility for transuranic chemistry; therefore, separation and analysis of transuranic isotopes and their radioactive decay products are important components of the portfolio. Knowledge of molecular-level processes is required to characterize and treat extremely complex radioactive mixtures in, for example, new nuclear fuel systems, and to understand and predict the fate of radioactive contaminants in the environment. Separations are essential to nearly all operations in processing industries and are also necessary for many analytical procedures.

Scientific Challenges

Challenges in separation science include the development of a deeper understanding of processes driven by small energy differences. These include self-assembly and molecular recognition, crystallization, dispersion, coalescence, and hysteresis in transport properties of glassy polymer membranes. The development of fundamental principles to guide ligand design for atomic and isotopic specific recognition and separations is also required. These, in turn, pose challenges to analysts to generate the understanding required to characterize amorphous materials through analysis of scattering data or other methods. Other analytical challenges include single-molecule detection and direct observation of bimolecular interactions and reactions. A deeper understanding of laser-material interactions as well as ionization and excitation sources for optical and mass spectrometric analyses is also required. Significant challenges are posed by elucidation of principles to underlie diagnostics at interfaces between synthetic materials and biomolecules, at oxide-aqueous interfaces, and to monitor spatial and temporal processes in and on the surfaces of living cells. Though understanding at the molecular level is required, there is currently insufficient knowledge to extend that understanding from the molecular level to the nanoscale, to mesoscale, and finally, to macroscale phenomena. Pursuit of that knowledge presents a major challenge to this activity.

This activity provides funding for about 50 university grants supporting, at any given time, on the order of 60-70 students and 25-30 postdoctoral fellows. In addition, 14 programs at national laboratories support numerous senior staff, and additional students and postdoctoral fellows. Programs at the laboratories are typically multi-investigator efforts on problems that require extensive collaboration by experienced scientists. These programs act as the focal point for specific research efforts vital to the DOE mission. This BES activity supports research programs at ORNL, Argonne National Laboratory (ANL), and Pacific Northwest National Laboratory (PNNL), with smaller efforts at Ames Laboratory, and Lawrence Berkeley National Laboratory (LBNL). Many of the research efforts at the national laboratories involve collaborations with the university and industrial communities.

Projected Evolution

Separations research will continue to advance the understanding of multifunction separations media; supramolecular recognition (using designed, multi-molecule assemblies to attract specific target species); synthesis of new porous materials and control of interface properties at the nanoscale; ligand design and synthesis of extractant molecules; mechanisms of transport and fouling in polymer and inorganic membranes; solvation in supercritical fluids; field-enhanced mixing; and drop formation.

Analytical research will pursue the elucidation of ionization and excitation mechanisms for optical and mass spectrometry; single molecule detection, characterization, and observation; nano- and molecular-scale analytical methods; laser-based methods for high-resolution spectroscopy and for presentation of samples for mass spectrometry; characterization of interfacial phenomena, with emphasis on chromatography; surface-enhanced Raman spectroscopy; and use of quadrupole ion traps to study gas-phase ion chemistry.

An expanded activity will support work to understand the underlying science needed to achieve true chemical imaging, i.e., the ability to selectively image selected chemical moieties at the molecular scale and to do so with temporal resolution that allows one to follow physical and chemical processes.