Research Activity: Engineering Research

Division: Materials Sciences and Engineering
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Portfolio Description:

Engineering Research advances scientific understanding underlying the dynamic interactions of single and multicomponent solid and fluid systems. Research considers the behavior and interactions of fluids including organic, biological, and complex fluids with each other and with solid systems; the transport of energy on and within these systems; and the development of means to advance the characterization of these systems. Issues under consideration frequently span several orders of magnitude in length and time scales and range from atomic interactions to macroscopic behavior and subpicosecond chemical events to fatigue events that may take years to reach completion. Accordingly they present a considerable challenge to theory, computational simulation, and experiment. Questions of interest have included understanding and predicting the behavior of (1) nanoscale structures and systems, including those with biological components; (2) dynamics of fluids, especially multi-component and complex fluids, but also including heat transfer, solidification, and granular materials; and (3) interactions of phonons with interfaces, secondary phases, or micro- and nanoscale defects in solids.

Unique Aspects:

The program is closely linked with the materials and chemical science activities of BES. Engineering Research has played a unique role in the National Nanotechnology Initiative (NNI) and Hydrogen Fuel Initiative (HFI) to further the understanding of nano- and meso-structures, devices and systems; molecular machines; transport behavior to and within consolidated nano-particulate material; and the dynamic behavior of multiphase, complex and biologically inspired materials, high surface area materials, consolidated nano-particulate materials, dispersion and coatings, photonics, nano-devices and molecular machines using nano-scale building blocks. This activity has had a leadership role in the fundamental understanding of multiphase fluid flow, heat transfer, and the fundamental behavior of granular materials.

Relationship to Other Programs:

Department of Energy (DOE)

- Office of Nuclear Energy Science and Technology (NE) - Nuclear Energy Research Initiative
- Office of Environmental Management (EM) - Environmental Management Science Program

Other Federal Agencies:

- National Science Foundation (NSF) – Exploring the possibilities of a joint initiative on neural electronics
- Interagency Working Group on Nanotechnology (NSTC/CT/MatTec)
- NSF, Department of Defense (DOD), and National Aeronautics and Space Administration (NASA) – Joint funding of research on Molecular Motor
- DOE representative on the Interagency Quantum Information Science Coordinating Group (NSTC/CT)
- Interactions with the community through: (1) workshops, such as the Workshop on Multiphase Fluid Flow, May 2002, and the Symposium on Computational Approaches to Disperse Multiphase Flows, October 2004; and (2) program presentations to the American Society of Mechanical Engineers, the American Society for Engineering Education, and other groups.

Significant Accomplishments:

- Assisted in creating an energy efficient chemical industry by developing databases, estimation techniques, and design models. ASPEN Tech was founded using these tools and now has over 1500 employees worldwide.

- Oil and gas companies are using results of research for more efficient transport and exploration of crude oil and natural gas. The Syncrude pipeline would not have been built without these developments that results in a 97% saving in energy used to transport the crude.
- Research on micro and nano systems has resulted in the developments of a nanosized biological motor for use in MEMS and NEMS devices
- Research on nanomotion from biomolecular interactions has led to the development of instruments for detecting and identifying molecules
- Adding small quantities of carbon nanotubes to a fluid dramatically increases its ability to conduct heat; however, theory predicts an even larger increase in conductivity. Experiments and simulations point to poor thermal coupling between the nanotubes and the fluid with implications for designing advanced heat transfer systems. Nanofluids have been created that conduct heat ten times faster than predicted possible.
- The thermal conductivity of single crystal silicon nanowires has been discovered to be two orders of magnitude lower than the bulk thermal conductivity of silicon. This is highly desirable property for thermoelectric applications. Simultaneously, the results reveal their limitation highly undesirable for many electronics and photonics applications.
- Record of heat flux dissipation has been achieved with a micro-channel two-phase flow (27,600 W/cm^2)

Mission Relevance:

New and improved understanding of dynamic behavior capabilities at the nano- and microscale will improve materials properties through improvements in processing and quality techniques, increased computing speed, improved sensing and control capabilities, further understanding leading to accurate predictions of materials and systems behavior, and enable larger-scale applications of devices with nano-scale components. Together these advances will further lead to higher process efficiency and lower energy consumption. Improving the knowledge base on multi-components fluid dynamics and heat transfer will have a major impact on energy consumption, because these phenomena are an integral part of every industrial process. Potential impacts include improved efficiency of fossil and nuclear based power generating systems.

Advances in non-linear dynamics will lead to improved control and predictive capabilities of complex systems, thus resulting in higher efficiency and lower energy consumption.

Scientific Challenges:

Focus areas include: accurate modeling of the transport of hydrogen and heat through nanoscale materials, and nanoporous and mesoporous structures; the understanding of anomalous thermal behavior of nanofluids and nanowires; understanding where continuum approximations break down in multicomponent systems containing fluids; describing, simulating, and engineering macroscale systems to take advantage of nanoscale behavior. Challenges also include understanding: (1) the potential of chemical and biological systems to construct complex, nanostructured materials under ambient conditions; (2) the role of interfaces and structure on the behavior of simple and complex fluids; (3) how more realistic sized groupings of drops and bubbles interact with each other and with their environment; (4) the mechanics and energetics of molecular mechanical devices, thus providing the foundations for their eventual use; (5) simple and complex systems driven far from thermodynamic equilibrium; and (6) the interactions of phonons with defects and interfaces.

Challenges in engineering sciences include identifying those scientific discoveries within the BES program that are most appropriate to pursue within the context of the energy and environmental mission needs of DOE, while supporting developments of engineering principles that enable scientific breakthroughs to be used for:

- Changing processes so that engineered systems are more energy efficient and environmentally friendly.
- Developing mathematical models of systems that can be used to make them better.
- Understanding the limitations of systems and extend those limits

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
5,306	2,444	1,000

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

Projected Evolution:

Shifts in research priorities and corresponding decreases in budget mandate an orderly completion of ongoing activities.