R & D facts

U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

Computational and Basic Sciences

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NETL's Onsite Research

As the lead field center for the DOE Office of Fossil Energy's research and development program, the National Energy Technology Laboratory has established a strong onsite research program conducted by Federal scientists and engineers who work closely with employees of contractor organizations and researchers from universities. Onsite R&D – managed by NETL's Office of Research and Development – makes important contributions to NETL's mission of implementing a research, development, and demonstration program to resolve the environmental, supply, and reliability constraints of producing and using fossil resources.

Researchers in NETL's Office of Research and Development perform onsite R&D in support of NETL's technology lines and for external government and industry customers. In addition, NETL's onsite research pursues knowledge, science, and technology with broad societal and industrial interest. NETL onsite R&D helps industrial and academic partners solve problems that would otherwise become barriers to commercializing power systems, fuels, and environmental and waste management technologies. NETL uses a variety of partnership mechanisms to conduct R&D of mutual interest with academic and private-sector organizations. The Office of Research and Development provides DOE's Fossil Energy program an onsite "corporate laboratory" at NETL. The onsite R&D efforts utilize state-of-the-art capabilities and facilities in Morgantown, West Virginia; Pittsburgh, Pennsylvania; and Albany, Oregon. About one-fourth of NETL's approximately 1,100 Federal and contractor employees are involved with onsite research activity. NETL is DOE's only government-owned, government-operated national laboratory; the onsite research program has a core group of about 150 Federal scientists and engineers. Supplemental site support comes from contractors who are selected through a competitive process, as well as research fellows and associates at the faculty, postdoctoral, graduate, and undergraduate levels.

Onsite research is conducted in four primary focus areas: Computational and Basic Sciences, Energy System Dynamics, Geological and Environmental Systems, and Materials Science.

Computational and Basic Sciences Focus Area

The focus area has developed a strategy to assemble computational models from *ab initio* (atomic and molecular) through device-scale, and to integrate the device-scale models into virtual plant simulations. In concert with this modeling work, experimental R&D is conducted in selected program areas in close, often iterative, collaboration with the computational efforts.

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Focus Area Research

The scope of the focus area research includes: quantum mechanical simulations, multiphase flow simulations, device-scale simulations using computational fluid dynamics (CFD), advanced process engineering co-simulations (APECS), integrated virtual plant modeling, hydrogen technology research and development, natural gas hydrates research and development, validation testing at each scale, and energy infrastructure security and interdependency analysis. The focus area supports activities in coal power systems and natural gas and oil technologies. It also strives to meet national energy security goals, including future technologies that can be used in a FutureGen prototype.

The long-term objective of the focus area is to provide the underlying science, engineering and computational foundations necessary for the environmentally friendly, highly efficient energy systems of the future. This area will:

- Develop the capability to accurately and robustly simulate reactive, heavily-loaded, gas/particle flows using methods of computational fluid dynamics
- Support DOD in its efforts to have a specification approved for a fully synthetic jet fuel for military applications
- Produce a technology base for robust, sulfur-tolerant, hydrogen separation membrane materials for coal gasification syngas streams
- Conceive and make available a suite of materials tailored to meet DOE goals for gas separations, storage and high-temperature applications in coal gasification, gas separations and fuels synthesis that will facilitate DOE objectives for the hydrogen economy and FutureGen
- Demonstrate an APECS steady-state FutureGen application that exploits advanced co-simulation, reduced order modeling, parallel solution, and virtual engineering
- Prototype APECS dynamic simulation capabilities
- Demonstrate FutureGen power plant simulation employing CFD device-scale models
- Develop the capability to design tailored materials using *ab initio* computational methods in conjunction with laboratory experiments