



the **ENERGY** lab

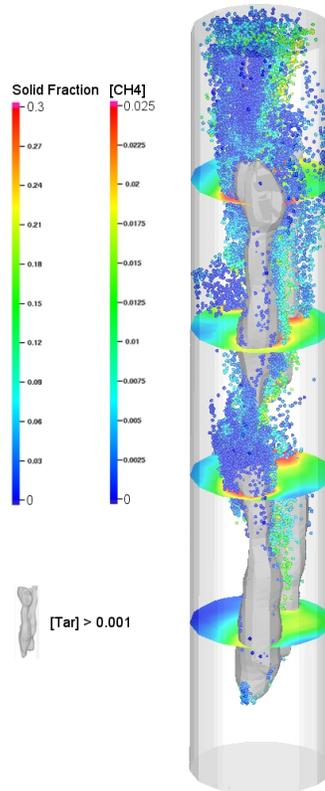
R&D FACTS

Computational and Basic Sciences

## Computational and Basic Sciences Onsite Research

As the lead field center for the DOE Office of Fossil Energy's research and development program, the National Energy Technology Laboratory (NETL) 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.



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**NATIONAL ENERGY TECHNOLOGY LABORATORY**

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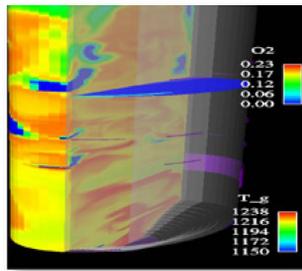
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U.S. DEPARTMENT OF  
**ENERGY**

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



## Computational and Basic Sciences Focus Area

The Computational and Basic Sciences Focus Area develops physics-based simulation capabilities for reducing the cost and time required for developing zero-emission energy systems, the simulation capabilities ranging from the particle-scale, to the device-scale, and to the plant-scale, generating information beyond the reach of experiments alone by integrating experimental and computational sciences across different length and time scales.

### Focus Area Research

**Reacting Multiphase Flow:** NETL is a recognized world leader in developing and applying computational fluid dynamic (CFD) models of reacting multiphase flow. Central to this capability is NETL's computational fluid dynamic code MFIX, open-source software with over three decades of development history and thousands of registered users worldwide. NETL is leading an effort in quantifying the uncertainties in multiphase CFD calculations so that the results can be used with confidence for scaling up reactors.

**Chemical Kinetics Data:** NETL developed the Carbonaceous Chemistry for Computational Modeling (C3M) software to provide direct links between reliable sources of kinetic information (kinetic modeling software, databases, and literature) and commonly used CFD software such as MFIX, FLUENT, and BARRACUDA with minimal effort from the user.

**Process synthesis, design, and optimization:** NETL develops and applies computational tools for optimal process synthesis, design, operation, and control of advanced energy systems.

**Multiscale modeling:** With its award-winning software product APECS (Advanced Process Engineering Co-Simulator), NETL enabled the coupling of process-scale models with device-scale models, including CFD models and fast reduced order models based on CFD results.

**Carbon Capture Simulation Initiative (CCSI):** The CCSI is an NETL-led partnership among national laboratories, industry, and academic institutions to develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the commercialization of carbon capture technologies from discovery to deployment.

**Dynamic and Real-time Modeling:** NETL's world-class Advanced Virtual Energy Simulation Training and Research (AVESTAR™) Center is built around a portfolio of high-fidelity, real-time dynamic simulators with full-scope operator training systems and 3-D virtual immersive training systems deployed in integrated energy-plant and control-room environments.

**Simulation-Based Engineering User Center (SBEUC):** The SBEUC supercomputer currently ranks as the 55th fastest computer in the world. It enables computational scientists at NETL to use high-performance computing to solve problems and accelerate energy technology development.

