COMPUTATIONAL SCIENCE & ENGINEERING
RESEARCH

NETL
NATIONAL ENERGY TECHNOLOGY LABORATORY

OVERVIEW

The U.S. Department of Energy's (DOE) National Energy Technology Laboratory's (NETL) Computational Science & Engineering (CSE) Directorate is recognized for its ability to develop science-based simulation models, mathematical methods and algorithms, and software tools required to address the technical barriers in the development of next-generation energy technologies. This competency works in collaboration with the other capabilities at NETL to generate information and scientific understanding beyond the reach of experiments alone through the integration of experimental information with computational sciences across different time and length scales.

R&D224, February 2019

The CSE Directorate is organized into three research teams that collectively maintain NETL's computational science and engineering competency:

- The *Computational Materials Team* maintains expertise in the modeling of materials at the atomic, molecular, and microstructural scales, which enables a fundamental understanding of materials behavior and provides insight into subsequent materials development opportunities and optimization strategies.

- The *Computational Device Engineering Team* maintains world-class capabilities in developing multiphase computational fluid dynamics models required for predicting the performance of fossil energy devices, such as advanced combustion reactors, gasifiers, emissions capture, and carbon dioxide (CO_2) capture units. The team has unique capabilities for linking models at multiple scales to increase the fidelity of the simulations.

- The *Data Analytics Team* is an emerging capability for developing and using data science methods to gain scientific insight from complex, high-dimensional, high-volume data sets from experiments and simulations conducted in support of energy technology development. The team uses machine learning to advance energy technology development.

Combined, these capabilities leverage world-class facilities to enable NETL's simulation-based engineering approach for accelerating the development and deployment of novel fossil energy materials, processes and device designs.

RESEARCH FACILITIES

- **Joule 2.0** is currently being installed and is designed to be a 5.62 PFLOP (one quadrillion floating-point operations per second) supercomputer that enables the numerical simulation of complex physical phenomena. Joule 2.0 will be used to run modeling tools at various scales ranging from molecules to devices to entire power plants and natural fuel reservoirs.

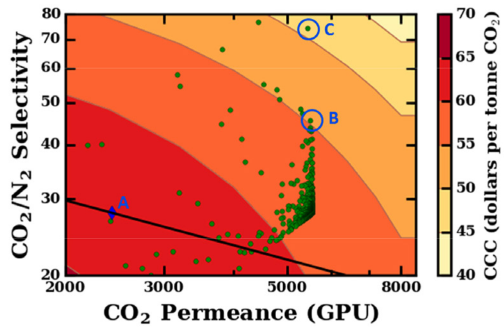
- **The Data Analytics Center of Excellence** allows NETL to explore problems in machine learning, artificial intelligence, data mining, and data analytics. The Center is specifically designed to house, move, and process multiple petabytes of data using a variety of cutting-edge algorithms developed in-house and with NETL's corporate and university research partners.

- **Visualization Centers** enable NETL researchers to visualize massive amounts of data in Pittsburgh, Pennsylvania; Morgantown, West Virginia; and Albany, Oregon.

USING CAPABILITIES TO SOLVE PROBLEMS OF NATIONAL IMPORTANCE

CSE allows research to be conducted that experimentation alone cannot achieve. These capabilities support research projects across all five NETL directorates, including diverse applications such as optimizing fuel cells, simulating/modeling complex gasification and combustion reactors, and predicting separations performance of materials for lower-cost carbon capture and more efficient extraction of rare earth elements.

High-Throughput Computational Modeling to Accelerate Materials Development. NETL demonstrated a high-throughput computational methodology to identify promising mixed-matrix membranes (MMM) for gas separations, such as for post-combustion carbon capture. Mixed-matrix membranes based on NETL Polymer 3 could decrease the cost of carbon capture from $63 to $48 per tonne of CO_2 removed.



	CO_2/N_2 Selectivity	CO_2 Permeance (GPU)	Cost of Carbon Capture
A: Pure Polymer	28	2421	$63
B: Predicted MMM	45	5494	$52
C: Predicted MMM	74	5440	$48

Figure 1. NETL research indicates that MMMs based on NETL Polymer 3 could decrease the cost of carbon capture.

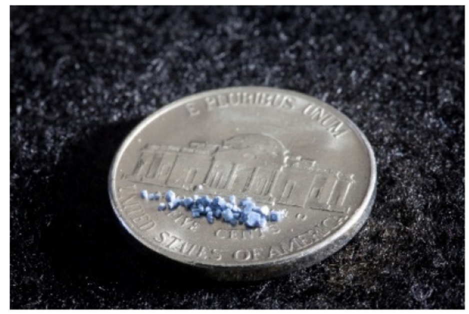


Figure 2. Metal organic framework materials have small porous holes that can selectively adsorb CO_2 over other gases.

ExtremEMat: NETL-Led National Laboratory Consortium to Accelerate Development of Extreme Environment Materials

NETL explores next generation crosscutting computational and experimental toolsets focused on accelerating discovery and scale-up of extreme environment materials. NETL demonstrated the application by using computational modeling tools to gain a fundamental understanding of the formation of high-entropy alloys (HEAs) and their properties and by developing high-performance HEAs for high-temperature fossil energy applications. This enables a next-generation crosscutting computational and experimental toolset focused on accelerating discovery and scale-up for reliably manufacturing materials at scale.

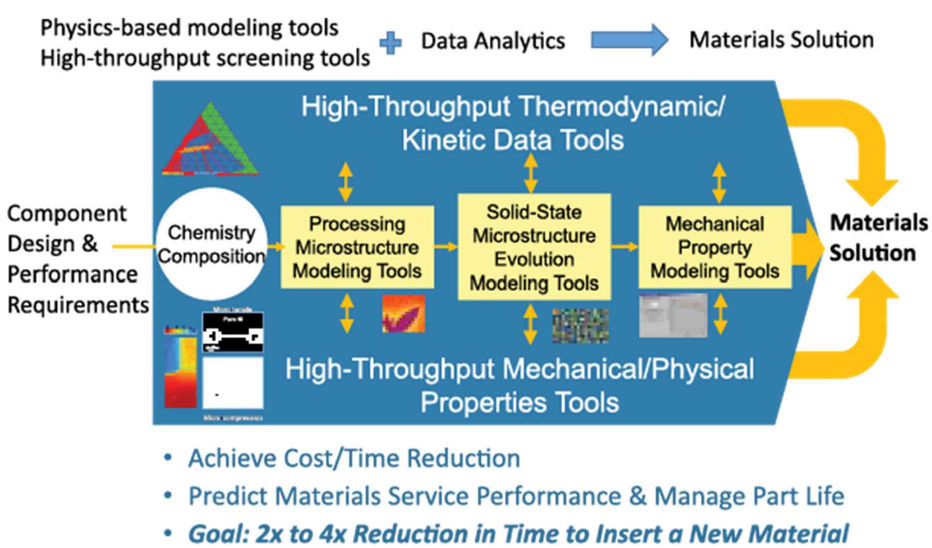


Figure 3. NETL's CSE capabilities reduce the time and costs associated with the material design cycle.

Multiphase Flow with Interphase eXchanges (MFiX): Open-Source Software Simulates Multiphase Flow Processes

MFiX is a suite of multiphase computational fluid dynamics (CFD) code developed specifically for modeling reacting multiphase systems. This open-source suite of software tools has more than three decades of development history and more than 5,000 registered users worldwide. This software has become a standard test bed for comparing, implementing, and evaluating multiphase flow constitutive models and has been applied to a diverse range of applications involving multiphase flows.

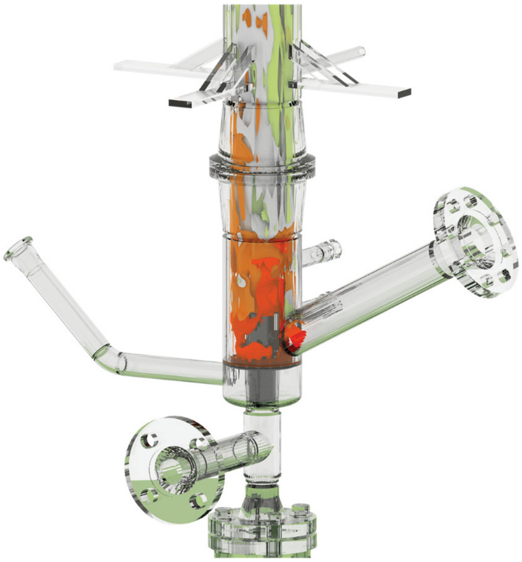


Figure 4. Coal gasification technology modeling using the multiphase CFD software portfolio.

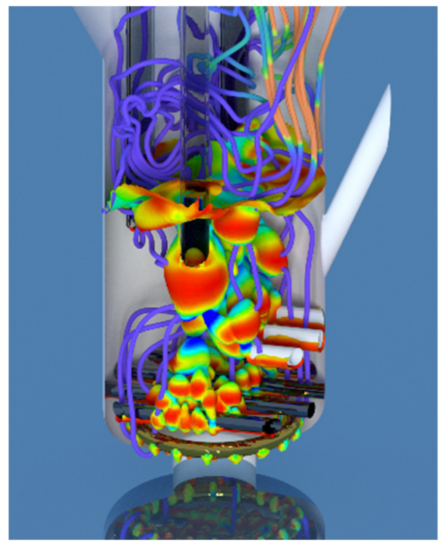


Figure 5. Researchers at the Idaho Nuclear Technology and Engineering Center at the Idaho National Laboratory are using simulations to better understand how well the waste and bed material mix, and how mixing in the vessel affects the performance.

NETL Partnership with Exascale Computing Project to Target Acceleration of Energy Technology Development

NETL, Lawrence Berkley National Laboratory, and the University of Colorado Boulder are conducting a multi-year effort that will enable NETL's open-source code MFiX to run on exascale computers. The project is supported by the Exascale Computing Project, a collaborative effort of DOE's Office of Science and National Nuclear Security Administration. This effort will increase the scale and speed capabilities of MFiX, enabling it to simulate with higher fidelity reactors used in fossil energy technologies. The simulations will help reduce the risks, costs and time required for scaling up laboratory designs to industrial sizes, while maximizing the benefits of high-performance computing for U.S. economic competitiveness.

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