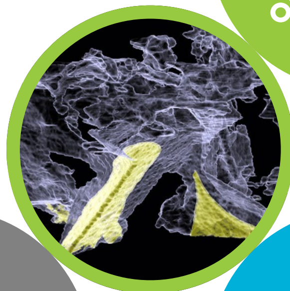
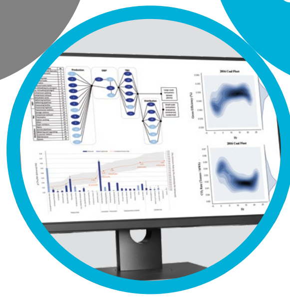
NETL Research &
Innovation Center

Directorates & Teams





NATIONAL
ENERGY
TECHNOLOGY
LABORATORY

Computational Science and Engineering (CSE)

NETL's CSE Directorate capability leverages three focus areas: computational materials engineering; computational device engineering; and artificial intelligence and machine learning. The simulation-based engineering approach accelerates development and reduces deployment costs for novel energy materials, processes, and system designs. Applications support across all the R&D activities and include cybersecurity for energy infrastructure, energy system assessments, component modeling, and material informatics.

Computational Materials Engineering

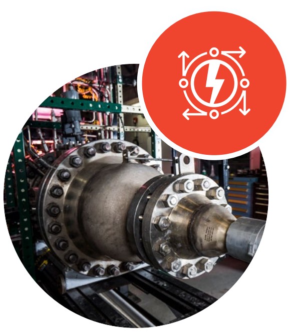
The Computational Materials Engineering Team maintains expertise in the modeling of materials at the atomic, molecular, and microstructural scales, which enables a fundamental understanding of materials behavior and provides insight into subsequent materials development opportunities and optimization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

Computational Device Engineering

The Computational Device Engineering team supports the collaborative development and application of Computational Fluid Dynamics (CFD) software and associated software tools. The purpose of these activities is to apply cutting edge CFD simulation tools to investigations of energy and carbon management technologies that will minimize the environmental impact of fossil fuels and contribute to meeting the national goal of net-zero greenhouse gas emissions. Emphasis is placed on the simulation of complex multiphase, reacting flows using supercomputing resources for the development, optimization, and troubleshooting of novel chemical reactors and other multiphase devices for advanced energy conversion and environmental applications. Our CDE researchers develop algorithms and computational software for high performance computers, including Exa-scale computers, and have access to NETL's Joule2 supercomputer.

Advanced Computing and Artificial Intelligence

The Advanced Computing and Artificial Intelligence 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.



Energy Conversion Engineering (ECE)

NETL's ECE Directorate conducts applied research to advance chemical conversion technologies. These capabilities are currently focused on development of hydrogen/ammonia storage and utilization; catalysts for microwave/plasma and electrolysis conversion of waste streams, fuels, and chemicals; chemical looping for carbon capture; separation systems for hydrogen, oxygen, and CO_2 including direct air capture (DAC); and the integration of energy components and systems to support grid resilience; and laser diagnostics.

Thermal Sciences Team

The Thermal Science Team conducts scale-up research for energy related technologies ranging from power to chemicals. As such, the team focuses on three capability areas: Reactor Design, Power Systems Science and Engineering, and Electrochemistry.

The Reactor Design capability focuses on heterogeneous solid-gas reactors such as circulating fluidized beds, bubbling fluidized beds, moving beds, spouting beds and risers for energy and chemical production systems such as fluidized bed reactors needed for DAC systems, gasification and chemical looping processes. solid fuel (fossil, wastes and biomass blends) in combustors or gasifiers or solid catalyzed gaseous conversion performance in methane pyrolysis reactors (examples: chemical looping, methane reforming, and Transport Reactor Integrated Gasifier) and related emissions reduction in multiphase contactors (examples: Dry Scrubbers and DAC).

The Power Systems Science and Engineering capability focuses on high pressure and temperature gaseous fuel (hydrocarbons, hydrogen and ammonia) oxy-combustion. (Examples: Supercritical carbon dioxide (sCO_2) Combustion and Pressure Gain Combustion) In addition, there is related heat transfer research such as sCO_2

heat exchanger and aerothermal blade cooling and combustor-turbine coupling for these advanced systems. The Electrochemistry capability focuses on high temperature electrochemistry for power generation and energy storage. Critical to these technologies is extending their lifetimes to help reduce costs, and the team holds both experimental and modeling capabilities to support these efforts.

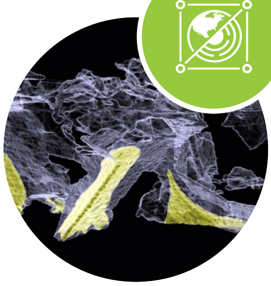
Advanced Systems Integration Team

The Advanced Systems Integration Team develops new methods and addresses applied problems in the integration and control of advanced systems for production of low-carbon power and hydrogen, such as hybrid power systems, magnetohydroynamic used in topping cycles, waste plastics and municipal solid waste gasification, and hybrids with energy storage. Much of the team's research efforts are to help address the dynamic control problems that are more prominent with increasing penetration of wind and solar onto the power grid, as well as in microgrids (common in industrial and other commercial applications) where generators require frequent load following capability.

The team applies methods including multiphysics simulation, dynamic system simulation, artificial intelligence, and cyber-physical systems to address these difficult problems. The approach taken for system integration usually has emphasis on leveraging or developing advanced controls and novel sensing capabilities and leveraging system integration benefits to maximize efficiency along with operational flexibility.

Reaction Engineering Team

The Reaction Engineering Team advances catalytic and energetic-supported reactor technology for production of valuable chemical and energy products, doing so efficiently and in an environmentally friendly manner. Examples are the application of electromagnetic fields, such as RF, microwave, plasma, etc., in the support of chemical transformations. The team performs scientific studies using various reactor environments to explore and elucidate reaction mechanisms, yields, kinetics, surface reactions, product yields, etc. The team provides a core capability of various reactor types and conducts analysis for energy conversion applications across a wide range of chemistry and separation processes. The Reaction Engineering Team leads the Center for Microwave Chemistry and provides nationally recognized leadership in microwave-enhanced reaction systems and microwave-assisted fuel conversions, both of which are essential for decarbonization and electrification of industrial processes. Additionally, the team provides leadership in water management, advancing the affordability, reliability, sustainability, and resilience of water in the energy sector.



Geologic and Environmental Systems (GES)

NETL's GES Directorate focuses its R&D capability to monitor, analyze, and predict the physical, chemical, and biological characteristics of complex surface, subsurface, and offshore environments. GES areas of research include gaseous storage; critical minerals; fractured formations and hydrates; monitoring of natural system behavior; geochemistry and geomicrobiology of produced waters; well integrity; geospatial data management and assessment; and methane emissions detection.

Geochemistry Team

The GES Geochemistry Team conducts research in subsurface geochemistry and geomicrobiology, mineralogy, resource assessment, techniques to monitor fluid-rock interactions, and reactive transport processes. The team studies physical effects of energy-related natural resource development and environmental mitigation strategies on natural and engineered geologic systems. The team also addresses key issues for critical mineral resource assessment, recovery tactics, and an overall strategy to create a critical mineral supply chain from domestic resources. The team employs world-class NETL facilities for fluid chemistry analysis, isotope analysis, microbiological DNA sequencing, subsurface process analysis, geomaterials characterization, cement and wellbore integrity investigations, and studies in high-pressure water environments. Additionally, the team develops new tools and processes to evaluate biological, chemical, and physical processes in geologic environments.

Reservoir Engineering Team

The GES Reservoir Engineering Team offers competencies in the characterization of hydrologic and geomechanical properties on natural and analogue cores or man-made specimens under single and multiphase flow situations with varying in situ temperature and stress conditions. The Reservoir Engineering Team seeks to better understand subsurface fluid flow and alterations of reservoir components. With this knowledge, researchers provide an enhanced capability to predict the behavior of reservoir responses to resource acquisition and fluid injection scenarios. Researchers develop and refine reservoir scale 3D models or ML-assisted reduced-order models to simulate responsive behavior of reservoirs, seals, and other subsurface systems upon resource utilization and exploitation utilizing NETL developed fractured reservoir modeling software, the National Risk Assessment Partnership's (NRAP) tools, and the Thermal-Hydrological-Chemical-Mechanical (THCM) reservoir simulator for methane hydrate production.

Geo-Analysis and Monitoring Team

The GES Geo-Analysis & Monitoring Team has expertise in airborne, ground-based, and field detection and monitoring investigations; data mining and analysis; monitoring and modeling of air quality; quantification of methane emissions; geophysics research; spectral imaging and remote sensing; tracers; geospatial mapping, analysis, and interpretation; and data analysis using statistical methods, artificial intelligence and machine learning (AI/ML), where appropriate. The team performs characterization activities that support resource extraction and geothermal development; identifies, quantifies, and helps develop strategies to mitigate the potential environmental impacts from development of energy resources; performs characterization and modeling through a combination of geospatial and geotemporal approaches to data including the use of AI/ML and state-of-the-art visualization methods. The team provides a critical link between research, regulators, and industry professional responsible for the safe, efficient development of subsurface resources.

Materials Engineering and Manufacturing Team (MEM)

NETL's MEM Directorate excels in the ability to design, engineer, and evaluate materials in diverse size and time regimes. Functional and structural materials development focuses on the design, synthesis, physical characterization, and performance testing of the nanomaterials, polymers, porous sorbents, ionic liquids, electro-ceramics, advanced alloys, and advanced ceramics required for carbon capture, gas separation, solid oxide fuel cell , sensing, highly efficient energy systems, and hydrogen technologies.

Functional Materials Team

The Functional Materials Team (FMT) seeks to design, develop, and deploy advanced materials needed to enable efficient and sustainable carbon management surrounding modern energy platforms. These efforts focus on the design, synthesis, physical characterization, and performance testing of nanomaterials, polymers, porous sorbents, ionic liquids, catalysts, membranes, and electro-ceramics required for the next generation of carbon capture, gas separation, hydrogen production, CO_2 conversion, chemical looping, solid oxide fuel cells, chemical sensing, fuel processing, and carbon materials technologies. The FMT is supported by a full complement of chemical synthesis laboratories; vapor-phase deposition equipment for materials growth; crystallographic and electronic structure characterization tools; surface science, imaging, and analysis instrumentation; mineral processing and separation laboratories; membrane manufacturing and testing facilities; and sensor manufacturing and testing facilities.

Structural Materials Team

The Structural Materials Team seeks to develop cost-effective alloys and ceramic materials that can withstand harsh conditions for long service durations. These materials are needed to achieve our nation's goals by mid-century (e.g., hydrogen turbines, hydrogen pipelines, carbon dioxide pipelines, and gasification). Specialty alloys are also needed for the defense, aerospace, automotive, chemical processing, biomedical industries, and other fields. NETL utilizes an integrated computational materials engineering approach, which combines computational and experimental methods for translating materials science concepts into practical technologies. Key to this strategy are targeted experiments that evaluate performance in realistic service conditions and that demonstrate manufacturing at scales and by methods that can readily translate to industrial practice. NETL's Advanced Alloy Signature Center (AASC) maintains a variety of furnaces for manufacturing mission-critical alloys, including air induction melting, vacuum induction melting, vacuum arc remelting and electro-slag remelting. The AASC also includes equipment for thermomechanical processing (e.g., press forge, roll mills, extrusion press, and heat-treating furnaces). In addition, the Severe Environment Corrosion and Erosion Research Facility and related laboratories are available for understanding a material's response to environmental factors critical for improving the integrity and reliability of systems. Capabilities are maintained for examining corrosion and oxidation of materials at high temperatures and high pressures. The team also has capabilities for assessing mechanical performance, including fatigue crack-growth in hydrogen, creep testing, and fatigue testing.

Materials Characterization Team

The Materials Characterization team conducts research on structure=property relationships in necessary for understanding and improving materials performance. The team has expertise on all classes of materials and collaborates with the other MEM and RIC teams to develop materials to enable the nation's goal of net-zero carbon emissions by mid-century. The team maintains state-of-the-art analytical instruments and laboratories necessary for complete materials characterization. This includes optical microscopy, metallography, scanning electron microscopy with the energy dispersive x-ray spectroscopy, electron backscatter diffraction, transmission electron microscopy, confocal scanning laser microscopy, electron microprobe analyzer, x-ray diffraction with various stages and accessories, wavelength dispersive x-ray fluorescence spectroscopy, interstitial analysis, inductively coupled plasma mass spectrometry, inductively coupled plasma optical emission spectroscopy, laser ablation inductively coupled plasma mass spectroscopy, Fourier transform infrared spectroscopy, atomic force microscopy, x-ray photoelectron spectroscopy (with reaction chamber), Brunauer-Emmett-Teller surface analysis, thermogravimetric analysis, differential thermal analysis, differential scanning calorimetry, laser flash diffusivity, dilatometry, computed tomography scanning, micro-hardness tester, Carbon, Hydrogen, Nitrogen, Sulfur Analyzer (CHNS) Ion Chromatography, etc. The team also utilizes other DOE-user facilities for advanced materials characterization.

Strategic Systems Analysis and Engineering (SSAE)

NETL's SSAE Directorate develops advanced process systems engineering models and state-of-the-art computational tools enabling decision-making of complex, multi-scale systems. These are critical to providing market, regulatory, and technical intelligence to decision makers and enable comprehensive evaluation of the most complex energy systems from the sub-process to the global scale. The multi-criteria and multi-scale decision tools and approaches developed to provide this support include evaluations to process systems, process and cost engineering, resource and subsurface analysis, market and infrastructure analysis, and environmental life cycle analysis.

Energy Process Analysis Team

The Energy Process Analysis Team leads complex techno-economic analyses of emerging technical matters associated with evolving U.S. energy conversion systems and markets, including power generation, the production and use of alternative fuels (e.g., hydrogen), the application of carbon resources to produce useful products (including critical minerals), and a variety of industrial processes. The team's work is heavily focused on the capture of CO_2 from power and industrial applications, as well as novel CO_2 removal technologies such as direct air capture. The team leverages a deep familiarity with the energy sector; associated commercial, emerging, and concept-stage technologies; relevant literature; state-of-the-art process synthesis, modeling, and simulation tools and techniques; data and statistical analysis techniques; and capital cost estimation methods to produce novel insights and R&D guidance in support of the cost-effective, environmentally-benign use of domestic energy resources as part of a reliable and secure domestic energy infrastructure.

Process Systems Engineering Research Team

NETL's Process Systems Engineering Research (PSER) Team brings together domain expertise in engineering, operations research, statistics, and applied mathematics to support decision-making for the design and operation of increasingly dynamic and interconnected processes and systems. PSER leverages the Institute for the Design of Advanced Energy Systems (IDAES) process systems engineering computational platform which performs modeling such as conceptual design; steady-state and dynamic optimization; multi-scale modeling; uncertainty quantification; and automated development of thermodynamic, physical property, and kinetic sub-models from experimental data, applied to advance fossil energy systems. Applications range from supporting decarbonization of the U.S. power industry to developing the U.S. energy, water, and manufacturing systems of the future. Core capabilities are often distributed via open-source software releases (e.g., CCSI Computational Toolset, IDAES Integrated Platform, WaterTAP, PARETO), and include predictive physics-based modeling, process synthesis and conceptual design, process design and optimization, multi-scale surrogate modeling, market-informed technoeconomic analysis, uncertainty quantification, sequential design of experiments, and robust optimization. Such tools are routinely applied to maximize learning and reduce the technical risk associated with scaling-up new technologies. The PSER team also possesses deep expertise in digital twin development and dynamic modeling to explore operational feasibility and control. Such capabilities enable the development of processes that can meet the requirements of a broad range of future energy scenarios while minimizing the negative impacts to efficiency, environmental footprint, and component health.

Energy Systems Analysis Team

The Energy Systems Analysis Team (ESAT) assesses environmental impacts using systematic approaches, like LCA, to ensure that comparisons are made on equivalent bases. LCA allows decision makers to evaluate the consequences of policy, guides research, and identifies opportunities for improvement. It includes the environmental burdens of converting fuel to useful energy, infrastructure construction, extraction and transportation of fuel, and transport of the final energy product to the end user. ESAT's LCA method also includes life cycle costing, which applies cost metrics to the same boundaries as their environmental models. ESAT has applied LCA to fossil, nuclear, and renewable energy systems that produce electricity and liquid fuels. Results are used to inform research at NETL and evaluate energy options from a national perspective.

In addition, ESAT interdisciplinary analysts are responsible for resource assessment, carbon storage, energy infrastructure, and novel energy systems analysis. ESAT provides geotechnical and engineering expertise to better understand, delineate, appraise, and promote safe utilization of critical subsurface energy resources. The team develops analyses, data, and models that accommodate the multi-disciplinary scientific, engineering and techno-economic aspects needed for holistic subsurface energy resource evaluation. Products developed (stand-alone or integrated into part of a larger energy system evaluation) are critical for informing a multitude of key stakeholders on subsurface energy system performance, associated cost drivers, practical research avenues, environmentally safe solutions, and economically viable deployment options. The team has expertise in developing technologies related to onshore and offshore carbon transport and geologic carbon storage, enhanced oil recovery, methane hydrates, unconventional oil and gas operations, produced water production and management, critical minerals, rare earth elements, geothermal and hydrogen transport; and enabling optimization at multiple scales (project, reservoir, basin, and nationwide) with the ability to leverage data-driven machine learning approaches for predictive modeling. Team efforts are essential to ensuring a safe and sustainable energy future that aligns with NETL and DOE's mission.

Energy Markets Analysis Team

The Energy Markets Analysis Team (EMAT) evaluates the potential role for advanced technologies, being developed by NETL R&D, to be competitive in the future U.S. energy landscape, under varying factors including market forces, macroeconomic trends, or government regulations. Scenario analyses use macroeconomic models and various pipeline and electric grid infrastructure models for regional, national, and global focused analyses. EMAT's analyses cross all sectors of the energy delivery system including electricity, coal, natural gas, petroleum, hydrogen, and water. The team has expertise in assessing current and future trends regarding modernizing all segments of the electric grid; pipeline transportation infrastructure for natural gas, petroleum, and their products; bulk commodity transportation systems including rail and commercial waterway;

pipeline infrastructure for carbon dioxide and hydrogen; and associated and interdependent systems including energy storage. In addition, EMAT conducts studies to evaluate potential benefits of its programs to ensure that the R&D investments not only contribute to the achievement of U.S. DOE missions but do so with a significantly positive economic impact regionally as well as nationally. This includes accomplishing the energy justice goals and objectives defined by the department.

Research Partnerships and Technology Transfer (RPTT)

NETL's RPTT Directorate supports NETL and NETL staff in identifying, exploring, and securing opportunities to leverage NETL's core capabilities and competencies and transfer technology to the private sector for commercialization. RPTT carries out this mission through strategic engagement, collaboration, and partnership with domestic and international government organizations, national laboratories, academia, industry, and other private and public stakeholders. These efforts directly align with the Lab's mission to enhance the nation's energy foundation and protect the environment for future generations. RPTT is also responsible for identifying and securing the Lab's strategic partnerships projects (also known as "work-for-others") and intellectual property management activities. In addition, RPTT leads and manages special initiatives, such as the lab's Regional Workforce Initiative:

Regional Workforce Initiative (RWFI)

Focused on providing a platform for regional stakeholders to engage the laboratory and other federal agencies in collaborative workforce development efforts for the Appalachian region and the nation. These efforts complement energy and advanced manufacturing innovation and research by addressing the necessary workforce needs and gaps necessary to successfully commercialize and deploy energy technologies.

U.S. DEPARTMENT of ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

Contact

Research Partnerships & Technology Transfer
partnerships@netl.doe.gov

Locations

Albany, OR
1450 Queen Avenue SW
Albany, OR 97321-2198

Morgantown, WV
Collins Ferry Road
Morgantown, WV 26507-0880

Pittsburgh, PA
626 Cochran Mill Road
Pittsburgh, PA 15236-0940

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