"We're leveraging world-class supercomputing and neutron science resources to design and test novel alloys for fossil fuel plants."

Yukinori Yamamoto,
Materials Scientist

# Innovations for Fossil Energy

Oak Ridge National Laboratory (ORNL) has a rich history of scientific research supporting the nation's exploration, production, and use of abundant, domestic fossil energy. We focus on research and development of materials and sensors for extreme environments; modeling and simulation of subsurfaces; and technologies for carbon capture, use, and storage.

## Materials for Extreme Environments

- Cutting-edge materials for use in boilers, turbines, and heat exchangers for ultra-supercritical steam and supercritical carbon dioxide ($CO_2$) power cycles and solid-oxide fuel cells
- New alloys and coatings to enable safer, longer lasting, and more efficient power plant operation
- Detailed analysis of novel materials to assist with certification before first use in power plants
- Advanced manufacturing of new components for fossil energy production and use

## Carbon Capture, Use, and Storage

Carbon capture, use, and storage is a strategy to stabilize the increasing concentration of $CO_2$ in the atmosphere. Recent breakthroughs at ORNL include the following.

- Capturing $CO_2$ from ambient air and binding it in crystal form using a novel, low-cost material and method for permanent storage
- Directly converting $CO_2$ to ethanol in a high-yield process using a nanotechnology-designed catalyst
- Using tracers to study the transport of $CO_2$ injected into the subsurface at the Cranfield site in Natchez, Mississippi—a unique, real-world test of $CO_2$ storage
- Exploring the basic science of seal resilience in $CO_2$ leakage from belowground carbon sequestration sites
- Developing models to predict how quickly mineral reactions occur in response to $CO_2$ sequestration—important for long-term security of storage sites

**INNOVATING** materials and sensors for power plants

**ENGINEERING** sorbents, solvents, and membranes for $CO_2$ solutions

**DEVISING** advanced imaging algorithms to see subsurfaces

**MODELING** concepts with supercomputing to speed research

**MAKING** manufacturing improvements for new alloys

*ORNL scientists at the field site of a Texas oil and gas company.*

# SubTER Program

DOE's Subsurface Science, Technology, and Engineering Research and Development (SubTER) crosscut program brings together stakeholders from the fossil energy, geothermal energy, nuclear energy, environmental, and basic science focus areas.

- High-performance computing (HPC) and novel computational imaging techniques to better model and simulate the subsurface environment
- Neutron imaging and scattering techniques to understand multiscale hydrocarbon storage within reservoir rock, flow through porous and fractured geologic materials, and deformation of geologic materials
- Advanced materials to improve construction techniques for wells
- Materials and sensors that can withstand a harsh underground environment and allow for better reservoir characterization
- Mineral recovery from geothermal brines and produced fluids, including membrane, solvent extraction, ion exchange, and sorbent technologies

# Modeling Subsurface Power Generation Applications

Researchers at ORNL and other organizations use our HPC resources to model their work for faster results.

- Ramgen Power Systems testing of aerospace shock wave compression technology for gas compression systems such as $CO_2$ compressors. Efficient compression of $CO_2$ could significantly lower the high cost of carbon capture and storage.
- Simulating the first coal plant with near-zero emissions. In a project for the National Energy Technology Laboratory, ORNL simulated clean coal technology that would result in a combined-cycle, coal-fueled power plant with near-zero emissions of nitrogen and mercury and that would trap most $CO_2$. The modeling work helped avoid the cost of building expensive prototypes.
- Virginia Tech used ORNL's Titan supercomputer to study subsurface multiphase flows, providing critical information needed to evaluate the efficacy of $CO_2$ sequestration in a given location.

*Tennessee Valley Authority's Bull Run Fossil Plant, a pulverized-coal supercritical power station in Clinton, Tennessee.*

## DOE HPC4Materials Program

ORNL is leveraging its world-renowned expertise and capabilities in materials science and HPC to develop materials that can withstand extreme conditions such as extreme pressures; extreme temperatures; radiation; or chemical, environmental, or fatigue stress states as part of the US Department of Energy's new **High Performance Computing for Materials Program.** Goal: Better performing materials that can save fuel and maintenance costs and increase US economic competitiveness.

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