



the **ENERGY** lab

PROGRAM FACTS

Advanced Research

Coal Utilization Science Program

Description

The Coal Utilization Science (CUS) Program sponsors research and development (R&D) in fundamental science and technology areas that have the potential to significantly improve the efficiency, reliability, and environmental performance of advanced power generation systems that use coal, the Nation's most abundant fossil fuel resource. The challenge is for these systems to produce power in an efficient and environmentally benign manner while remaining cost effective for power providers as well as consumers.

The CUS Program is carried out by the National Energy Technology Laboratory (NETL) under the auspices of the U.S. Department of Energy's (DOE's) Office of Fossil Energy (FE). The program supports DOE's Strategic Plan to:

- Promote America's energy security through reliable, clean, and affordable energy.
- Strengthen U.S. scientific discovery and economic competitiveness.
- Improve the quality of life through innovations in science and technology.

Current research within the CUS Program targets the development of critical and enabling technologies that contribute to the design and operation of advanced near-zero emission power and fuel systems. These systems include the demonstration of multiple commercial-scale Integrated Gasification Combined Cycle (IGCC) or other clean coal power plants with cutting-edge carbon capture and storage (CCS) technology.

Advanced Research—To support coal and power systems development, NETL is opening new avenues to increase power plant efficiency, reliability, and environmental quality. NETL's Advanced Research Program conducts a range of pre-competitive research focused on breakthroughs in materials and processes, coal utilization science, sensors and controls, computational energy science, and other novel energy-related concepts. NETL also sponsors cooperative educational initiatives in University Coal Research, Historically Black Colleges and Universities, and Other Minority Institutions.

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Within NETL's Advanced Research organization, CUS performs a crosscutting function, serving as a bridge between basic science and the engineering of new technologies by identifying critical research needs and barriers, gaining a thorough understanding of the underlying chemical and physical processes involved, and developing the tools required to overcome those barriers.

Program participants use state-of-the-art methods to explore novel concepts, perform theoretical investigations, examine critical processes and mechanisms, and generate high-quality data.

CUS Program participants include businesses, universities, and other national laboratories. Flexible teaming arrangements enable multi-laboratory teams to cooperate both formally and informally. The generic and noncommercial nature of the research has led to international collaboration through the annex to the International Energy Agency Implementing Agreement on Clean Coal Science as a way of extending limited R&D budgets.

Program Focus Areas

NETL's CUS Program conducts research projects in the two primary focus areas described below. These areas address the more complex operational requirements of advanced coal plants, which are designed to be integrated with CCS subsystems.

Sensors and Controls Innovations — Novel sensors and advanced process control are key enabling technologies for advanced near-zero emission power systems. CUS is leading the effort to develop sensing and control technologies and methods to achieve seamless, integrated, automated, optimized, and intelligent power systems. The performance of advanced power systems is limited by the lack of sensors and controls capable of withstanding high temperature and pressure conditions. Harsh environments are inherent to new systems that aim to achieve high efficiency with low emissions. In addition, these systems are complex, with operational constraints and system integration challenges that push the limits of traditional process controls. As R&D enhances the understanding of these evolving advanced power systems, it is clear that new, robust sensing approaches, including durable materials and highly automated process controls, are needed to optimize their operation and performance.

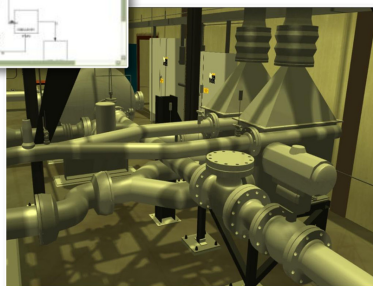
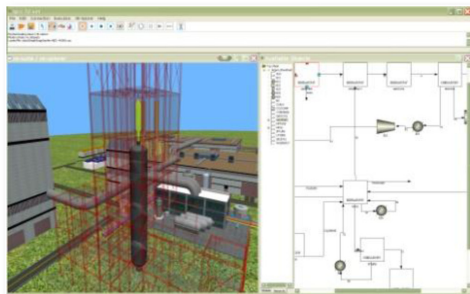
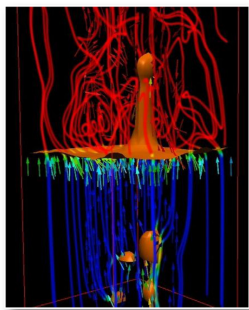
Computational System Dynamics — Simulating the complex processes that occur inside a coal gasifier, or across an entire chemical or power plant, requires a powerful tool made possible by today's supercomputers and advanced simulation software. The Computational System Dynamics focus area provides such tools to the CUS Program. The goal is to help scientists and engineers better understand the fundamental steps in this complex process so they can optimize the equipment needed to run it. This not only costs less, but also provides more information than a long series of experiments performed under varying conditions to try to isolate important variables. Of course, the data are only as good as the computer model; some of today's computer models have proven to be excellent when measured against as-built configurations.

Program Successes

CUS R&D has had numerous noteworthy successes achieved under Advanced Research's broad mandate to conduct research that supports the development of technologies for clean, efficient electric power generation. Success often is gauged by the ability to scale-up a technique or transfer a new technology or approach to the demonstration phase. In other cases, direct commercialization of the technology is a measure of success. With funding from NETL, for example, researchers at The Ohio State University developed a high-temperature oxygen micro sensor as part of a broad-ranging effort to more closely monitor total nitrogen oxides (NO_x), carbon monoxide (CO), and oxygen (O₂) during combustion. The oxygen sensor was selected by R&D Magazine in 2005 as one of the 100 most technologically significant products introduced into the marketplace over the previous year.

NETL Sensors and Controls R&D has yielded a number of additional successes to date, among them:

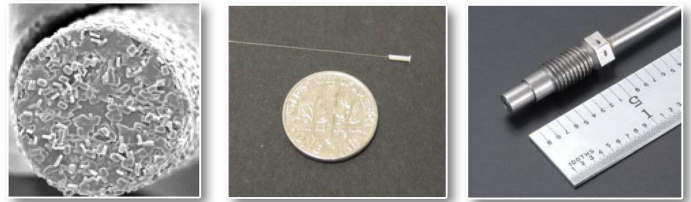
- A new, robust, accurate temperature measurement system that can withstand the harsh conditions found in commercial gasifiers for an extended period.
- Pilot-scale testing of a number of novel sensors to assess commercial feasibility, including fiber optic temperature and strain sensors, a silicon carbide optically-based temperature sensor, polymer derived ceramic sensors for 1000°C temperature detection in turbine environments, and high-temperature micro gas sensors in exhaust gas environments.
- First demonstration of the viability of constructing high-temperature, fiber-based gas sensors capable of selectively detecting gases at or near 500 °C, including nano-coated fibers for the detection of primary constituents in synthesis



VE-PSI helps overcome some of the hurdles in the current engineering workflow by enabling seamless integration of process simulation data into a comprehensive virtual engineering environment containing computer-aided design (CAD) data, computational fluid dynamics (CFD) data, and many other engineering data sources.

gas and modified porous silica fiber for rapid detection of low molecular hydrocarbons.

- A field-portable kit for screening halogenated volatile organic compounds from soil and water samples, providing a streamlined method for testing redevelopment sites for environmental contamination.



High temperature sensor materials, coatings, designs, and prototypes play key roles in creating novel measurement technologies for high temperature harsh environments.

Additional research in sensors and controls is underway to develop:

- A suite of high-temperature, harsh environment, sensors to measure temperature, pressure, and other process variables.
- Novel sensors to measure key properties and constituents in coal, natural gas, synthesis gas (e.g., hydrogen), flue gas constituents (e.g., NO_x), and trace contaminants (e.g., mercury).
- Advanced process control strategies for near-zero emissions in processes such as gasification and chemical looping.

Examples of successes in the Computational System Dynamics area include the following:

- **The Virtual Engineering-Process Simulation Interface (VE-PSI)** has won both an R&D 100 award in 2009 as well as Federal Laboratory Consortium (FLC) award for Excellence in Technology Transfer in 2010. The VE-PSI, an application used to access process simulator functionality within the Virtual Engineering Suite (VE-Suite), performs a unique integration function and provides engineers with the ability to review and revise proposed designs more quickly, more efficiently, and at less cost than ever before.

- **Multiphase Flow with Interphase eXchanges (MFIx)** software, internationally recognized as the pre-eminent software for modeling gas-solids (multiphase) flow, won an R&D 100 Award in 2007. MFIx works on optimizing one functional unit, such as a coal gasification reactor, at a time.
- **Advanced Process Engineering Co-Simulator (APECS)** software combines commercial process simulation and computational fluid dynamics to help industries design highly integrated plants. APECS won an R&D 100 Award in 2004 and a FLC Excellence in Technology Transfer Award in 2007. APECS coordinates many functional units across an entire plant to optimize its operational efficiency.

Continuing research in Computational System Dynamics focuses on:

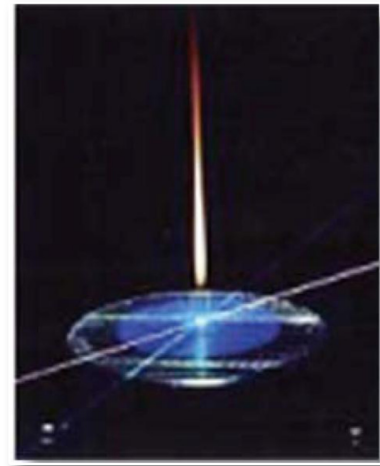
- Projects related to steady-state simulations, the framework that supports the simulations, the reduced-order models to carry out the simulations for reacting flows and carbon capture demonstrations.
- Integration of co-simulator models with virtual engineering plant walk-through environment models.
- Efforts to expand and validate multiphase fluid flow models for simulation of advanced coal-based power systems.
- Investigation of basic combustion and gasification chemistry to determine mechanisms that affect emissions behavior or coal under advanced and conventional combustion/gasification.

The computational system dynamics information is used to validate combustion/gasification models, enabling the use of the integrated modeling and simulation packages in the design and evaluation of advanced power systems, including those under development for carbon capture demonstrations.

Benefits

The CUS Program has produced important advances in the science of coal utilization. R&D under this program, for example, has led to the first one- and two-dimensional combustion-capable Computational Fluid Dynamics code in the U.S. The program also has provided insights into coal devolatilization, char reactivity, and ash behavior that have led to new mechanistic models used in several commercial

and research-oriented combustion codes. Many of today's low-NO_x burners and advanced re-burning technologies are based on the kinetic data and models developed through this program.



CUS projects are using laser diagnostics to probe the way coal burns.

These advances have translated to enhanced technology transfer and commercial availability through industrial participation, lower costs through reduction of initial investment and operating expenses, and the creation of new jobs and investment opportunities. Support for national research capabilities and facilities has enabled highly skilled scientists and engineers to promote fuel diversity and helped to maintain a competitive U.S. economy.

Additional Information

Additional information may be accessed electronically through the following link to the NETL Advanced Research Reference Shelf: <http://www.netl.doe.gov/technologies/coalpower/advresearch/ref-shelf.html>

