the ENERGY lab

Advanced Research: Innovation Leading to Successes

Exploring the "Grand Challenges" of Fossil Fuels

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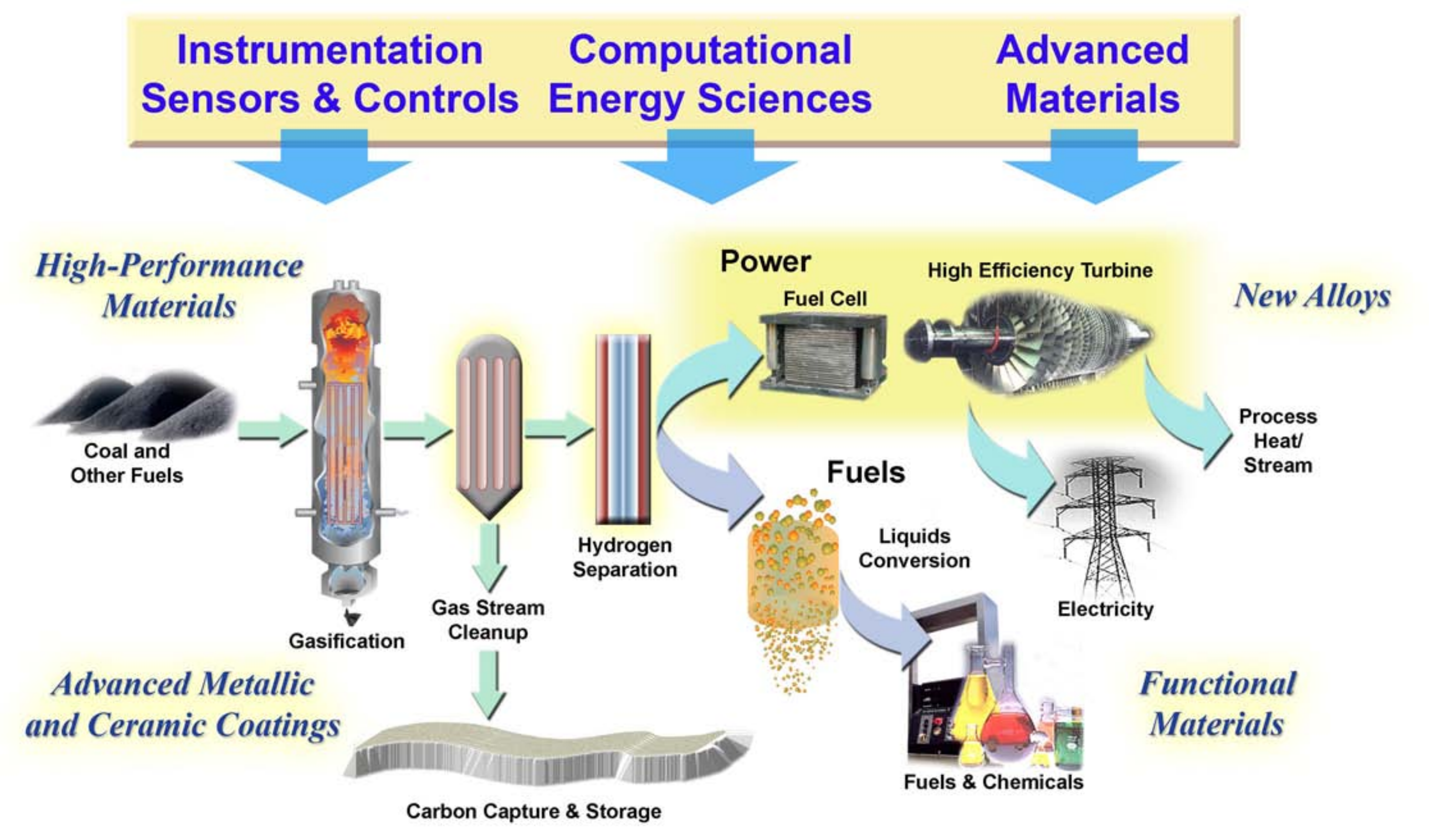
NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DEPARTMENT OF ENERGY

NETL Advanced Research

The Advanced Research (AR) Program *within the Office of Coal and Power Systems of the National Energy Technology Laboratory (NETL), the research arm of the U.S. Department of Energy's Office of Fossil Energy (DOE/FE), fosters the development of innovative, cost-effective technologies for improving the efficiency, reliability, and environmental performance of advanced coal and power systems. In addition, AR bridges the gap between fundamental research into technology alternatives and applied research aimed at scale-up, deployment, and commercialization of the most promising technologies identified.*

AR projects explore the "grand challenges" of fossil fuels— the barriers to more effective use of the nation's abundant domestic fossil fuel resources. Conducting fundamental, basic research for advanced fossil energy technologies, AR provides the first, fostering steps toward developing a variety of coal and power technologies. AR pursues projects in several key focus areas that are considered to be of greatest relevance and potential benefit to advanced coal and power systems. These areas include High-Performance Materials, Coal Utilization Science, Sensors and Controls Innovations, Computational System Dynamics, and Computational Energy Sciences. The common thread is the focus on breakthrough technologies or novel applications that strive to balance high risk against the prospect of high payoff.



"Enabling"—or breakthrough—technologies are designed to meet various goals, such as higher efficiency power generation, reduced transportation emissions from new carbon-based hydrogen storage media, and production of advanced ultra-clean synthetic transportation fuels. And novel concepts help speed the pace of technology innovation and "virtual" demonstrations of complex systems that are used to reduce overall research and development (R&D) expense. Through these efforts, NETL Advanced Research is spearheading research advances for DOE/FE, in close partnership with industry, universities, and other national laboratories.

AR manages a broad portfolio that includes pre-commercial projects that rely on NETL's in-house facilities and depth of expertise, as well as collaborative external arrangements that draw upon diverse outside resources. The AR program has an extensive reach, currently involving some 130 organizations from industry, academia, non-profit organizations, and other national laboratories in all but a handful of states across the nation.

Innovative materials

Lower emissions

Design optimization

CO_2 capture/use

Strategic benefits

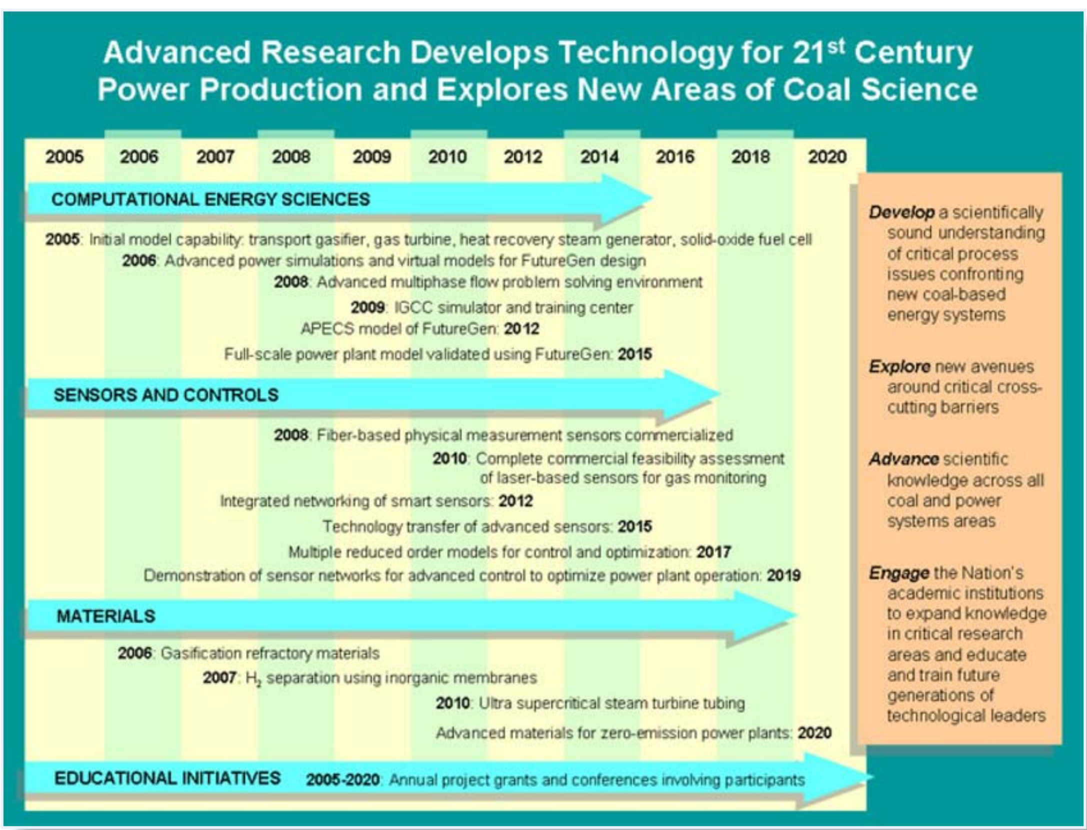
Ecological gains

Bio-waste reduction

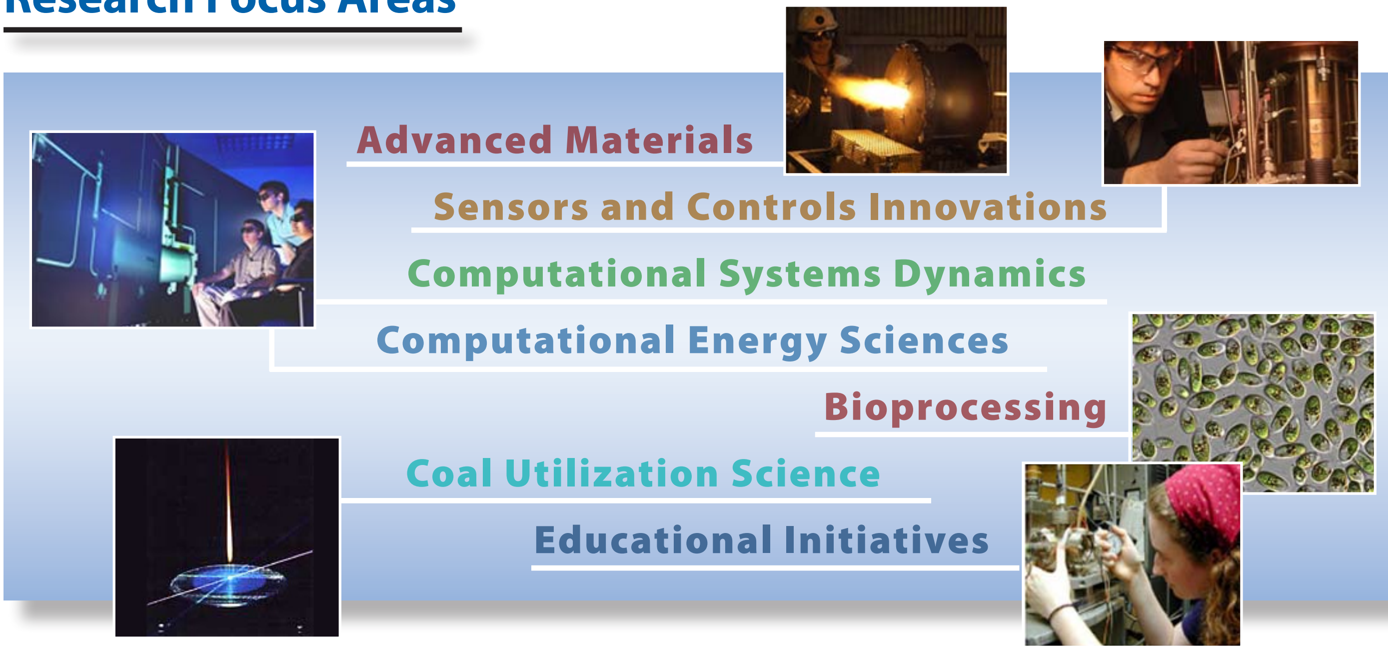
Process improvement

Greater efficiency

H_2 co-production



Research Focus Areas



***High-Performance Materials** are vital to enhancing the cost, performance, and success of fossil energy systems. The purpose of research in this area is to develop materials of construction, including processing and fabrication methods, and functional materials necessary for those systems.*

AR's High-Performance Materials R&D effort cuts across many scientific and technological disciplines to investigate properties of promising materials and to develop high-temperature, corrosion-resistant structural ceramic composites, alloys, and materials for specific functions in fossil fuel environments. The challenge is to develop materials having unique thermal, chemical, and mechanical properties. Areas of focus in this area currently are: High-Temperature Materials Research and Materials for Ultrasupercritical and Other Advanced Fossil Energy Power Generation Systems.

Materials research often is a risk taking effort where the probability of success sometimes *may* be low. However, the payoffs are potentially high and of great value to provide the critical supporting technology needed to achieve performance improvements for advanced, combined cycle and coal combustion systems, while at the same time eliminating materials having little or no promise.

Several such projects have led to important successes, laying the foundation for new strategic energy production that decreases both the nation's dependence on imported fossil fuels *and* emissions of greenhouse gases associated with fossil fuel use.

***Coal Utilization Science** is a crosscutting R&D effort whose goal is to expand the basic understanding of the underlying chemical and physical processes involved in utilizing coal in order to overcome the barriers to coal utilization.*

CUS research has produced important advances in the science of coal utilization. From CUS, for example, has come the first one- and two-dimensional combustion-capable Computational Fluid Dynamics code in the United States. CUS research also has provided insights into coal devolitization, char reactivity, and ash behavior that have led to new mechanistic models now used in several commercial and research-oriented combustion codes. Research in this area currently has two areas of focus: Sensors and Controls Innovations, and Computational System Dynamics. These areas address more complex operational requirements of advanced coal plants, which are designed to be integrated with carbon capture subsystems.

Sensors and Controls Innovations *research focuses on novel sensors and integrated process control, which are key enabling technologies for advanced, near-zero emission power systems.*

AR is leading the effort to develop innovative sensing and control technologies and methods to achieve seamless, integrated, automated, optimized, and intelligent power systems that improve the efficiency and enhance the reliability and availability of power systems. Researchers also are investigating more durable materials needed for sensors that can survive for an acceptable length of time in the harsh environments of advanced power systems.

Computational System Dynamics *research centers on advanced simulation techniques that enable more rapid development of advanced, highly efficient, low-emission power plants.*

AR projects in this area relate to steady state simulations, the framework that supports these simulations, and the reduced-order models to carry out the simulations. Information derived from this research is used to validate combustion/gasification models, thereby enabling the use of these integrated modeling and simulation packages to aid in the design and evaluation of advanced power systems such as those under development for carbon capture demonstrations.

Computational Energy Science *provides high-performance computational modeling and simulation R&D in advanced power plant design, speeding development and reducing costs of new technology development.*

AR is developing complex yet flexible computational tools that will allow for more rapid and efficient scale-up of new subsystems and components. These tools will be used to improve power plant operation and, most significantly, will reduce the need for large and expensive demonstration-scale testing of integrated energy systems through simulation, modeling, and computational resources. For example, advanced computational methods used to design FutureGen-type systems will be more cost-effective than conventional processes.

Some projects are developing critical components that are influencing the design of near-zero emission power plants. These projects include, for example, the capability to utilize interactive visualization technology to design next-generation power plants. Other projects are implementing advanced, distributed Computer Aided Design (CAD) tools for virtual design groups, primarily computer model development and simulations.

Other Related Research *provides important and award-winning innovations in multiple areas of fossil fuel use.*

As the AR program has evolved over the years, there are some important research efforts that no longer fit neatly into the key research focus areas. For example, Bioprocessing shifted its emphasis from more traditional types of research designed to change coal into a more desirable fuel, to more imaginative areas aimed at assisting power generation in overcoming persistent environmental problems. Much of the work in these other areas is in basic science and fossil fuel research in the areas of biology, biochemistry, microbiology, and bioengineering. AR fosters innovative uses for coal combustion by-products, development of alternative fuels, identification of biomass sources, and mitigation of environmental impacts from mining and fossil fuel use. AR also addresses environmental issues that affect the power industry, including development of biological greenhouse gas sequestration technologies.

NETL advanced research solutions promote convergence of energy production and use factors.

Pathways to Commercial Applications

AR activities differ somewhat from those of most NETL technology programs. The accomplishments from fundamental and basic AR research represent the initial steps en route to new, advanced technologies. These efforts feed into and support the more advanced systems research of individual technology programs within DOE/FE, from gasification to turbines and fuel cells, and new power plant modeling techniques. In the process, AR also makes other important discoveries—identifying project directions through fundamental research that prove not to be worth further investigation.

AR offers many business opportunities using a variety of NETL contract and funding vehicles. **Financial assistance vehicles** are used to support or stimulate R&D for a public purpose and include:

- ***Grants***, which are used when there is no need for substantial involvement between the recipient and agency during performance of the grant. Grants result from competitive proposals in response to solicitations.
- ***Cooperative agreements***, which are used when substantial involvement is needed between the recipient and agency during performance. Cooperative agreements result from unsolicited proposals submitted in response to Notices of Program Interest.

AR-specific academic and private sector research programs are discussed as follows.

Business Opportunities with NETL

FedBizOpps.gov and Grants.gov provide e-mail notification services to interested parties who want to receive information about the posting of an acquisition or financial assistance opportunity.

Register for acquisition opportunity notices at:
http://www.fbo.gov/EPSVendorRegistration.html

Register for funding opportunity notices at:
http://www.grants.gov/search/subscribeAdvanced.do

See NETL's designated business points of contact for more information about these opportunities.

***Educational Initiatives** have been providing opportunities since 1980 for collaborations between universities and NETL in many areas of fossil fuel research.*

The academic environment is well suited to fundamental research—with high payoff potential—that may lead to applied research and scale-up to commercial use. Involvement of professors and students is conducive to the generation of fresh ideas. In addition, student participation serves a vital national interest—ensuring the continuing availability of scientists and technologists with appropriate expertise for the U.S. energy industry. AR educational projects are aimed at helping the nation achieve its clean air and climate change goals, as well as helping boost domestic oil supplies.

The University Coal Research (UCR) Program provides grants to U.S. universities to support fundamental research that cuts across NETL's product lines, and develops improved fossil energy technologies. Its primary purpose is to improve the fundamental scientific and technical understanding of the chemical and physical processes involved in conversion and utilization of coal and coal by-products. Since these grants first became available, over $100 million has been provided and more than 1,700 students have acquired invaluable experience in understanding the science and technology of coal.

The Historically Black Colleges and Universities/Other Minority Institutions (HBCU/ OMI) Program provides a mechanism for cooperative research among HBCU/OMI institutions, U.S. industries, and Federal agencies. The central thrust of the program is to generate fresh ideas and tap underutilized talent, define applicable fundamental principles, and develop advanced concepts for generating new and improved technologies across the full spectrum of fossil energy R&D programs. The program also provides a forum to facilitate technology transfer, strengthen educational training, and develop and enhance the research infrastructure and capabilities of HBCU/OMI for producing the next generation of scientists and engineers of diverse backgrounds. It provides and promotes opportunities for HBCU/OMI in science and engineering within DOE/FE that foster private sector participation and interaction with HBCU/OMI in fossil energy-related programs.

AR Successes

There are many noteworthy instances where AR project efforts, once completed, have moved into larger-scale technology programs, and then on to commercial successes. It is these successes that are highlighted in the following pages—successes that have provided measurable benefits to coal and power systems technologies: improved efficiencies, lower costs, new materials, and new processes.

Spotlight on Success:

***Advanced Research** projects build bridges between basic research and the development and deployment of innovative systems that are capable of improving the efficiency and environmental performance of our nation's fossil energy resources—in particular, coal and power systems.*

An Integrated Hydrogen Production—Carbon Capture Process from Fossil Fuels

CHALLENGE: Separating H_2 and CO_2

SOLUTION: Re-form coal emissions

This innovative project was conducted in conjunction with Clark Atlanta University and Scientific Carbons, Inc., to produce hydrogen and fertilizer from coal and biomass using a pyrolysis-reforming process. The process also incorporated the capture of CO_2 from smokestack emissions, producing a carbon fertilizer. The ability to convert char from coal and biomass into both hydrogen and a slow-release fertilizer will facilitate the use of hydrogen as a clean source of energy. It simultaneously provides a way to sequester CO_2, a major greenhouse gas that contributes to the challenge of global climate change.

Pilot plant pyrolysis unit with biomass feedstack system.

Improved Refractory and Thermocouple Materials for Commercial Slagging Gasifiers

CHALLENGE: Short-lived materials

SOLUTION: Extend material lifetime

A crucial element in realizing the successful advanced, zero-emissions power plants of the future is the high-performance coal gasification system. Certain materials needed to construct refractory liners and thermocouple assemblies—key components of gasification systems—have unacceptably short service lives, limiting the efficiency, reliability, and cost-effectiveness of gasification. Through this project, AR was able to develop ways to extend the lifetimes of these materials.

Successful laboratory and field tests on improved refractory materials have validated that they will have much longer and more reliable service lifetimes than materials currently used. The extended lifetimes translate into possibly over one million dollars in annual operating cost savings, as well as a significant increase in gasifier online availability. This work was developed by NETL, and continued with industrial partners ANH Refractories Co./Harbison-Walker Refractories Co., ConocoPhillips Company, Eastman Chemical Company, and TECO Energy's Tampa Electric Company.

Laboratory test of refractory performance under extreme operating conditions.

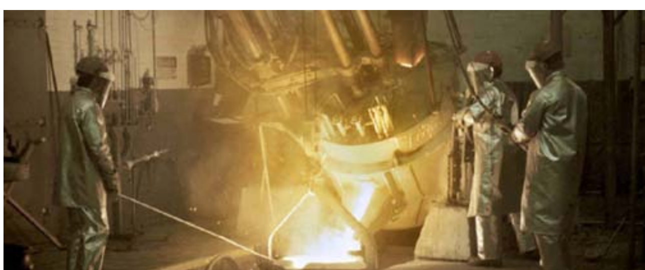
Addressing Materials Processing Issues for Steam Turbines: Cast Versions of Wrought Nickel-Based Superalloys

CHALLENGE: Increasing efficiency places greater demands on equipment

SOLUTION: Develop more robust materials for steam turbines

Steam turbines used in power plants with increased power production efficiency and reduced carbon dioxide emissions must be constructed with more durable materials capable of withstanding higher temperatures and pressures. Fabrication of turbines used in ultra-supercritical plants requires large castings with new, robust materials. Engineers at NETL are developing and testing new superalloys that withstand higher pressures and temperatures and can be cast under conditions required for fabricating large components.

Researchers examined a suite of traditionally wrought nickel-based superalloys cast under conditions designed to emulate the full-sized casting, including factors such as large pour weights, thick section components, and slow cooling rates. Small-scale castings of seven alloys and at least eight alloying elements were made for testing. Slow cooling was achieved by surrounding the mold with loose sand to simulate the conditions of turbine casing component casting. Grain-etched ingot cross sections were found to have grain structures similar to those expected in large sand cast versions of the alloys. Secondary dendrite arm spacing was measured to estimate local solidification rates on which to base heat treatment procedures. Data was collected for seven candidate alloys. Three alloys selected for further testing have been cast and are currently being evaluated. The results of heat treatment, creep, and other performance tests performed on these nickel-based superalloys show promise for their eventual use in ultra-supercritical power plant construction.



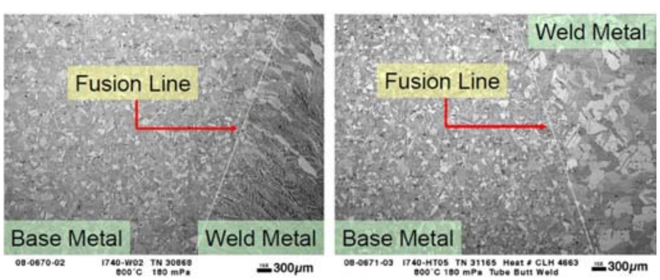
Casting a sample of one superalloy candidate from the melt crucible (top) into a mold designed to stay below 550°C (at right) to simulate the slow cooling that occurs for large castings.

Materials for Advanced Ultra-Supercritical Steam Boilers

CHALLENGE: Need to increase temperature and pressure

SOLUTION: Develop superalloys for boiler fabrication

Higher efficiencies for power production require increases in operating temperatures and pressures. This project conducted by Oak Ridge National Laboratory (ORNL) investigates alloys that may endure challenging conditions in steam boilers. Researchers examined precipitation-strengthened Ni-based superalloys placed under conditions designed to simulate the commercial use of the materials, paying specific attention to creep rupturing, weld strength, and cold-work limits. Researchers are characterizing creep behavior and mechanisms, identifying fabrication and welding issues, collecting creep data for boiler design efforts, and performing longer-term tests. Pressurized tube bend creep tests provide data to aid in determining cold-work limits and guidance for developing fabrication rules. Investigators are studying Weld Strength Factors, crystallographic images, weld microstructures, and cross-weld creep testing results. The tests will help determine which superalloys will be best suited for advanced, ultra-supercritical (AUSC) boiler fabrication. In addition, availability of these types of data will build confidence in the use of new materials for boilers in AUSC power plants.



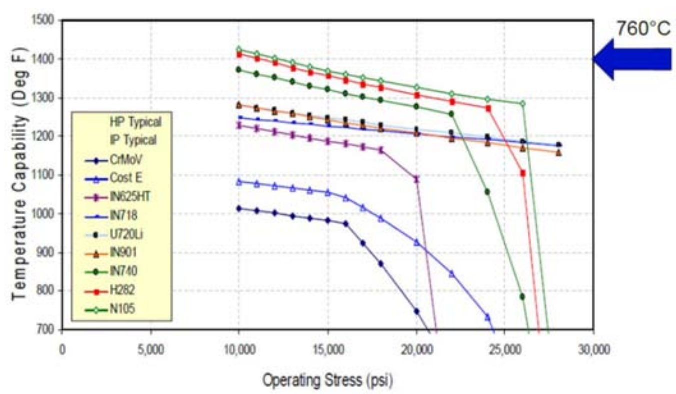
Weld microstructures can be modified by heat treatments. The weld on the left was aged at 800 °C for four hours and the weld on the right was solution annealed at 1120 °C for one hour before being aged at 800 °C for four hours.

Materials for Advanced Ultra-Supercritical Steam Service – Turbines

CHALLENGE: Require specialized materials

SOLUTION: Screen materials for potential

Continued increases in temperature and pressure in power plants are essential for increased energy production efficiency as well as reduction in emissions. Oak Ridge National Laboratory (ORNL) collaborated with NETL to cast and test a number of nickel-based superalloys to investigate their feasibility for use in the construction of turbines for ultra super-critical plants. Initial screening tests of a wide range of alloys at 800°C narrowed candidates to two to four alloys for each of three specific turbine applications. Researchers studied yield strength, creep-rupture strength, grain size, creep resistance, rupture ductility, temperature capabilities, and homogenization to characterize superalloys with respect to possible use for advanced, ultra-supercritical (USC) steam turbine component fabrication. The project will continue with weldability testing and development of materials for use at the commercial scale.



A graph of temperature capabilities of nickel-based superalloys shows two alloys outperform the rest for high-pressure or intermediate-pressure rotor application.

Development of Continuous Silicon Carbide Composites

CHALLENGE: Strengthen structural ceramics

SOLUTION: Unique reaction bonding process

The EERC has been developing and testing high-temperature materials for advanced power systems, as part of NETL's efforts to improve efficiency and reduce emissions from fossil energy systems. In one of many subtasks, EERC developed a new process for making continuous microporous silicon carbide (SiC) composites. This process has potential applications in diverse fields from power generation systems to automobile engines to spaceflight.

The unique reaction bonding process developed by EERC produced SiC that maintained its strength to at least 1,450 °C, which is much higher than any other reaction bonding technique. The material also is approximately 35 percent porous, allowing it to be infiltrated with a second phase such as a polymer or a metal to make a stronger composite. This unique method allowed for the creation of near-net-shape, continuous but porous SiC composites.

To determine whether the SiC composite would be stable for long periods in space while exposed to intense ultraviolet radiation (and atomic oxygen in low-earth orbit), eight coupons of the material were included with others in the Materials International Space Station (ISS) Experiment No. 6 (MISSE-6) and launched on the Space Shuttle Endeavour on March 11, 2008. They will remain in orbit approximately one year, during which time they will make 6,000 orbits and travel 150 million miles before being retrieved during a future Shuttle mission and returned to Earth for analysis.

Photo of deployed MISSE experiments taken from the Space Shuttle Endeavour (photo courtesy of NASA).

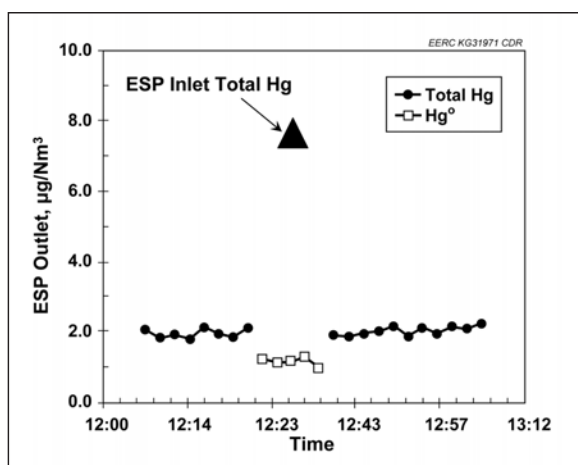
Inorganic Coal Additive for Controlling Mercury Emissions and Mitigating Slagging and Fouling

CHALLENGE: Capture mercury emissions

SOLUTION: Optimize inorganic coal additive

Energy Efficient Combustion Technology (EECT) teamed with the EERC to further develop EECT's noncarbon-based mercury (Hg) control technology. Under this project, the EERC is developing inorganic additives for capturing Hg that are specifically tailored to key parameters related to coal chemistry and that avoid potential ash-handling issues. The challenge is to capture low concentrations of various forms of mercury within seconds. Currently, mercury is captured from flue gas in scrubbers or by using various sorbents upstream of particulate control devices. The levels of performance are mixed, depending on coal type, flue gas constituents, and plant configuration.

The new EECT–EERC technology addresses these shortcomings by providing a solution that is environmentally friendly, effective at removing both elemental and oxidized forms of mercury, and usable in many flue gas streams that would normally poison activated carbon sorbents. The EERC has physically and chemically modified EECT's inorganic additive technology and performed bench- and pilot-scale optimization to achieve significant Hg removals from the combustion of a high-ash-content and low-Hg-content subbituminous coal. Electrostatic precipitator (ESP) Hg removal efficiencies of 72–76 percent were obtained on the high-ash, high-alkaline subbituminous coal combustion flue gas during the injections of EECT additive into the furnace, as indicated in the figure.



Continuous mercury monitoring during the injection of EECT additive into a coal combustion flue gas.

Novel Oxygen Supply Process

CHALLENGE: Better combustion needed

SOLUTION: Replace air with oxygen

Oxygen is proving to be a good alternative to air for burning fossil fuels such as coal in an oxy-fuel combustion-based power plant. Oxygen-fueled combustion results in a highly pure exhaust stream that can be captured at relatively low cost and stored in a variety of ways. For example, oxycombustion technology may provide the means to capture greenhouse gases, including CO_2, at existing coal-fired power plants. To develop this improved process, AR joined forces with Wyoming’s Western Research Institute (WRI) to develop a pilot-scale test facility and perform operational testing of an innovative process for oxygen production and supply using recycled flue gas. The tests were very successful and yielded heating and combustion data that will be used in further demonstrations to advance the process toward commercialization. Reducing the cost and technical risk of oxycombustion technology will help move the nation closer to cleaner, more efficient power generation from coal, the nation’s most abundant fossil fuel resource.

Compressors and carbon dioxide unit at WRI pilot-scale test facility.

Halogenated Volatile Organic Compound (HVOC) Field Screening

CHALLENGE: Need to test for HVOCs in the field

SOLUTION: Develop portable screening tool

Prior to expansion or redevelopment of industrial sites, developers must test the soil and water for environmental contamination, including HVOCs. Since such tests usually are costly and time-consuming, developers have sought ways to streamline the testing process. Through this innovative project, AR has been working with WRI and Bacharach, Inc. to develop and commercialize the X-Wand®, a new field-portable kit for screening HVOCs. This research has led to development of new, cost-effective commercial technology to rapidly screen for HVOCs in the field. This is an important time-and-cost-saving solution for analytical laboratories, since screening can now be performed in minutes rather than by a full, costly exploratory analysis of an extra sample.

X-Wand® analyzer rapidly screens for HVOCs in the field.

New Soil Volatile Organic Compound (VOC) Sampler

CHALLENGE: Improve VOC sampling

SOLUTION: Standardize and enhance methods

Under this jointly sponsored research project, AR has been working with WRI and a VOC sampler developer, ESI Chem, Inc. over the past decade to improve and commercialize a sampler called the En Core® Sampler. During this time, the team has been developing validating methods to collect and screen surface-level soil samples for VOCs in field applications using the sampler. Furthering this research, WRI has worked in turn with En Chem, Inc., and their manufacturing subsidiary En Novative Technologies, to develop and achieve approval by the ASTM (American Society for Materials and Testing International) of a standardized test methodology to be used in connection with the En Core® Sampler. This project expanded the scope of research and began developing a new subsurface soil sampler, the Accu Core™ Sampler, which can be used to collect soil samples down to 180 feet below the surface. En Novative has sold more than 30,000 of the En Core samplers, and provides royalties to WRI based on the sales.

Above, an attachable, reusable En Core® T-handle is used to push the sampler into the soil.

SO_3 Emission Control Technology for Coal-Fired Power Plants

CHALLENGE: Reduce SO_3 gas emissions

SOLUTION: Inject fine particles to condense the SO_3

The EERC, along with Marsulex Environmental Technologies and the AlstomPower Inc. Air Preheater Company, has been working to develop solutions to sulfur trioxide (SO_3) emission problems in coal-fired boilers. A significant pollutant in its gaseous form, SO_3 is the primary agent in acid rain and a precursor to sulfuric acid (H_2SO_4).

The basis of the SO_3 reduction technology being demonstrated by the EERC and its partners is to provide controlled condensation of SO_3 by injection of fine particles immediately upstream of the air preheater (APH). The condensation process does not depend on the composition of the particles, but only on the particle-size distribution and particle concentration. Limestone was chosen for its low cost and its ability to provide a degree of acid neutralization after condensation has occurred.

A computer model developed by the EERC determined the amount of SO_3 transformations and interactions across an APH to assist in developing strategies to minimize the level of SO_3 released to the environment. The results of the modeling work indicated a significant reduction of SO_3 in the presence of fine particles less than approximately 5 µm in diameter as the flue gases containing SO_3 passed through the APH and ductwork upstream of the ESP. The model predictions were corroborated by early field observations during demonstration at a full-scale utility boiler. This finding provided a unique opportunity to reduce the level of SO_3 in the flue gas as it passes through an APH.

Validation of Fireside Performance Indices Using PCQUEST

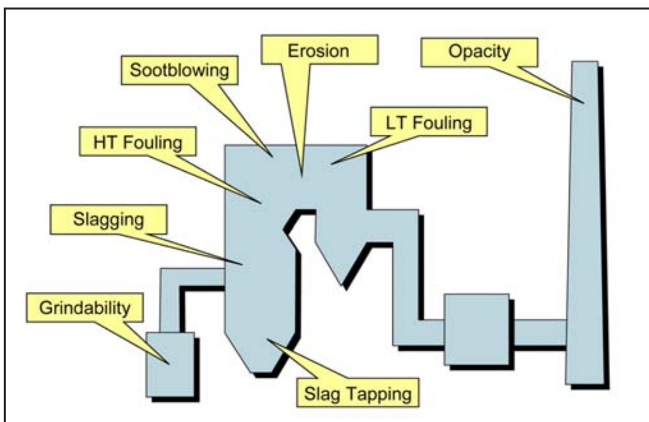
CHALLENGE: Match coal fuels to boilers

SOLUTION: Validate using computer model

Using its previously developed PCQUEST predictive computer model, the EERC—in collaboration with NETL and numerous industry partners—has developed a fundamental knowledge base on how ash deposits form inside (i.e., on the "fireside" of) coal-fired combustion boilers and how the composition of coal inorganics leads to ash deposition. PCQUEST was built to predict the severity of furnace wall slagging, high- and low-temperature convective pass fouling, slag-tapping ability, tube erosion, and opacity for conventional pulverized or cyclone-fired coal combustion systems, as shown in the figure below.

The goal of the most recent research was to validate, improve, and provide commercial utility for the predictive indices contained in PCQUEST, so that utilities and coal companies could identify the best coals for their equipment to optimize power plant efficiency. The project involved first quantifying organically associated elements in coal using chemical fractionation (CHF) and discrete minerals using computer-controlled scanning electron microscopy (CCSEM). The types of fly ash and ash deposits that form are temperature- and boiler zone-dependent.

Real-world problems faced by several utilities, coal companies, and other industries have already been mitigated or solved using PCQUEST, saving these industries in some cases up to $350,000 annually for a 500-MW boiler.



PCQUEST indices are derived from coal combustion performance characteristics.

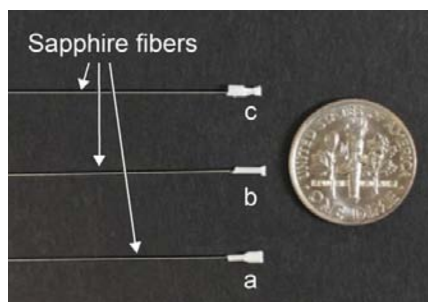
Single-Crystal Sapphire Optical Fiber Sensor Instrumentation

CHALLENGE: Gasifier too harsh on sensors

SOLUTION: Develop new sensor material

The Center for Photonics Technology at the Virginia Polytechnic Institute and State University (Virginia Tech) has developed a new, robust, accurate temperature measurement system that can withstand the harsh conditions found in commercial gasifiers for an extended period, thus allowing improved reliability and advanced process control. Through this AR project, a sapphire-based fiber sensor head provides temperature data from inside the gasifier at temperatures up to 1,600 °C using an extrinsic Fabry-Perot interferometric sensor. The prototype sensor was subjected to a full-scale field performance demonstration in a Tampa Electric Company gasifier at Polk Power Station in Florida. Initial testing was very successful—the sensor lasted three times as long as current technology.

Development of a single-crystal sapphire temperature sensor that can accurately measure gasification conditions in such harsh conditions will increase the reliability and efficiency of gasifier systems. Gasifiers are central to many advanced high-temperature power systems, including integrated gasification combined-cycle (IGCC) systems. Tomorrow's advanced power generation systems such as FutureGen will benefit from this development. Other high-temperature applications may benefit as well.



Single-crystal sapphire sensor heads with sapphire fiber waveguides achieve greater precision through miniaturization.

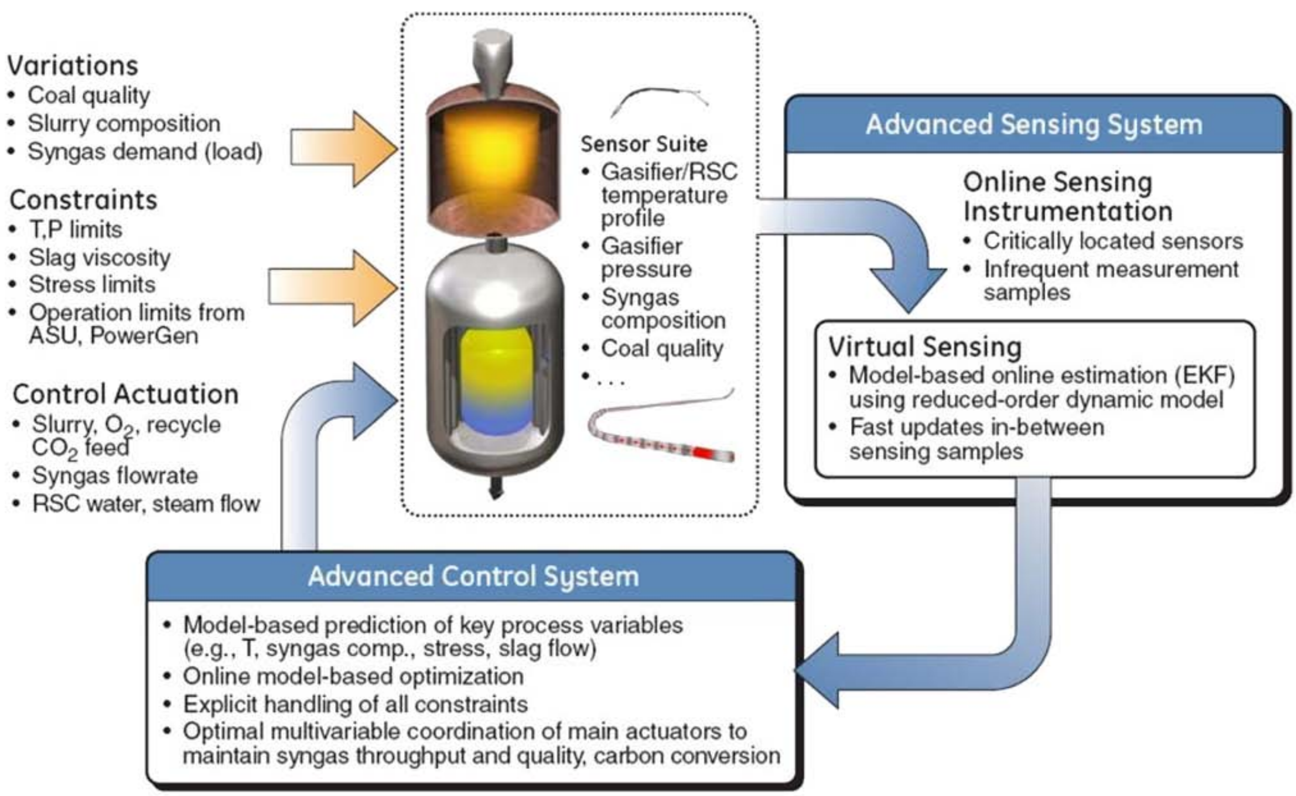
Development of Integrated Model Based Sensing and Control Solution for Entrained Flow Gasifiers

CHALLENGE: Create advanced sensing and control strategies to improve the operation of the gasification section in an IGCC plant.

SOLUTION: Implement a set of model-based estimation and control algorithms for improved operation of the gasification section in an IGCC plant during startup and normal operation.

Gasification offers a viable pathway to cleanly generate power and fuel and is a cost-effective option for carbon dioxide sequestration. However, certain technology areas of the gasification process require innovative advanced control algorithms to enable the system to perform as intended. General Electric (GE) Global Research and GE Energy in conjunction with the National Energy Technology Laboratory (NETL) have developed an integrated sensing and control solution, employing nonlinear model-based estimation and model predictive controls to achieve improved availability, efficiency and operation flexibility.

To address this key limitation, the researchers developed an integrated advanced sensing and control solution, coupling available limited online sensors with a nonlinear extended Kalman filter and model predictive control in Matlab/Simulink® environment. The researchers validated the performance of the developed sensing & control solution using extensive simulations with sensor and modeling errors. The studies showed potential for significantly faster startup and more efficient and flexible operation at steady state as well as during load and fuel changes with coal and coal-petcoke blend fuels.



Overall Integrated Sensing and Control Solution coupling online sensors with model-based estimation and control.

Combustion Control and Diagnostics Sensor (CCADS) for Advanced Gas Turbines

CHALLENGE: Need *in-situ* combustion control

SOLUTION: Develop heat-resistant sensor

As progress has been made toward advanced turbines that can operate on coal-derived synthesis gas, AR has focused research on developing new means for precise fuel delivery. The CCADS project is considered a breakthrough technology that can provide turbine manufacturers the capability to detect and control combustion dynamics, leading to higher efficiencies and dramatically lower emissions.

A key requirement for gas turbines — achieving fuel-lean homogenous mixing of the fuel and air in all combustion zones — is also a prerequisite to operating syngas-ready turbines at required emission levels. The CCADS research project was aimed at developing a simple multi-sensing yet robust, *in-situ* monitoring sensor to diagnose combustion conditions and activities. NETL developed and patented this innovative sensor for gas turbines and has licensed it to industrial partner Woodward.

Integrating CCADS electrodes into the existing premixed fuel nozzle eliminates the need for extra ports in the combustor wall—a requirement that, until now, has limited acceptance of online combustion monitoring by turbine manufacturers due to both added complexity and expense. In addition, the CCADS electrodes are manufactured from the same high-temperature alloys as the premix nozzle, so they are resistant to the high temperatures and pressures at the combustor inlet. The sensor is able to monitor flame properties such as fuel/air ratio and flame stability, facilitating more precise control of combustion.

CCADS use with feedback control will increase turbine stability over the entire operating range and result in higher performance, durability, and lower emissions. Electric utilities will benefit through reduced costs for maintenance and emissions penalties. CCADS also can be retrofitted to existing turbine installations to provide additional operating flexibility.

CCADS has a very low cost relative to the total cost of a turbine while also providing substantial benefits both to turbine manufacturers and utilities. The market potential for advanced nozzles incorporating CCADS is conservatively estimated at tens of thousands of units per year in both new installations and retrofit markets. Eliminating unwanted combustion dynamics could result in an estimated $1 billion per year cost savings, and this number could increase with future implementation of IGCC with advanced turbine systems.

NETL engineer inspects the CCADS installation in the SimVal rig section.

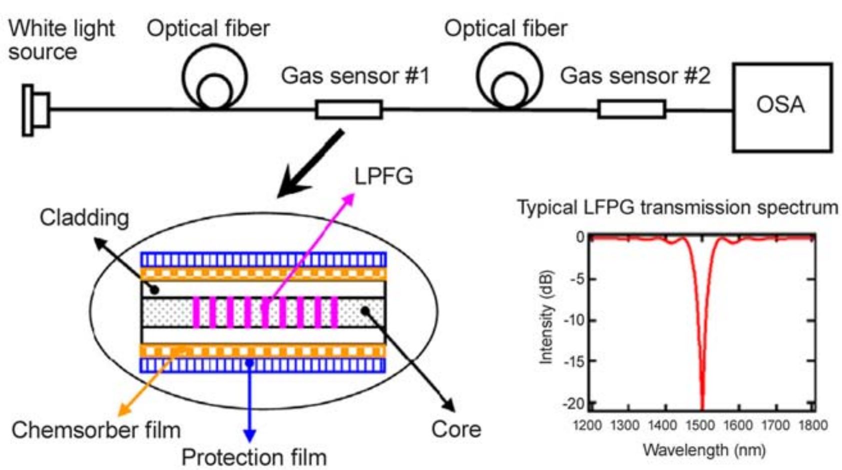
Nanocrystalline Doped-Ceramic-Coated Optical Fiber Gas Sensor

CHALLENGE: Advanced Power System Generation in a Harsh Environment (extreme temperatures, pressures, corrosive atmosphere, erosive particles)

SOLUTION: Develop new sensor material

New Mexico Institute of Mining and Technology lead electrochemical engineering researchers at the University of Missouri Science and Technology (formerly Rolla) and the University of Cincinnati to develop a new type of sensor suitable for in situ and fast gas monitoring (>500 °C) by coating silica-based optical fibers with nanocrystalline-doped ceramic materials. The films detection of hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), and hydrogen sulfide (H_2S) are well suited for the concentrations and conditions found in the production and treatment of syngas, the product of gasification.

The primary technology (shown in the figure below) demonstrates the commercial viability of multiplexed fiber optic-based micro-sensors for distributed gas detection of the nanomaterial-coated thermal long-period fiber grating (LPFG)-based high-temperature gas sensors. Consequently, the networking of these gas sensors will enhance advanced process controls contributing to high efficiency, high reliability, and outstanding environmental performance of existing and future advanced power systems.



Schematic illustration of nanomaterial-coated thermal long-period fiber grating (LPFG)-based high-temperature gas sensors.

High Temperature Sensor Suite and Adaptable Sensor Packaging

CHALLENGE: Sensing in High Temperature Gas Stream

SOLUTION: Ceramic Based Micro Sensor for Combined Temperature and Pressure Measurement

Sporian Microsystems, Inc. has developed the *first* Silicon Carbide Nitride (SiCN) ceramic multi-sensor suite capable of measuring temperature and pressure on a single chip and in a high temperature (+1000 °C and high pressure (up to 1000 psi) environment. Through Phase I and Phase II Small Business Innovative Research Grants (SBIR), Sporian has successfully developed the SiCN material and materials processing in collaboration with the University of Central Florida. Additionally, significant developments in sensor suite design and sensor packaging have been completed and successfully demonstrated at the pilot scale.

The sensor is based on a polymer derived ceramic (SiCN). This versatile material can be doped to resist corrosion, change the conductivity of the material, and to enable its operation at very high temperature. Because the material is derived through a polymer process, it can be made into dense thick films, thin films or as bulk porous material. This versatility also enables the sensor to be packaged using the same material as the sensor thus eliminating the failure mechanisms due to dissimilar materials under harsh conditions (e.g. coefficients of thermal expansion).

Sporian is continuing to develop the sensor technology for DOE, other government agencies, and for private industry. The work has rapidly progressed from fundamental material studies through successful demonstration of integrated sensor device. Sporian plans to commercialize the technology after long term demonstration of the sensors is complete. Through other grants, Sporian has also been able to demonstrate durable operation of the sensors for over 250 hours in a combustor rig at temperatures near 600 °C and have also modified the SiCN material to enable survivability of the sensor at temperatures near 1300 °C. Packaging improvements such as robust die attachment, high pressure sealing, porous screens and electrical interconnection techniques have also been achieved which allow the packaged sensor or probe to operate at sustained temperatures of 1000 °C with excursions to 1200 °C.

The ability to sense pressure and temperature under challenging conditions within a power plant, combustion and steam turbines, as well as aero turbine machinery will directly contribute to operational performance of the system and efficiency of the unit. An in-situ pressure sensor would allow improvements in gas turbine efficiency and a reduction in emissions by allowing the turbine to safely operate closer to the surge line of the turbine without adverse effects. The sensor suite can also reduce down time and maintenance; temperature spikes and pressure-related phenomena such as 'rumble' and 'screech' shorten the mean time to repair and mean time to failure in these expensive assets.

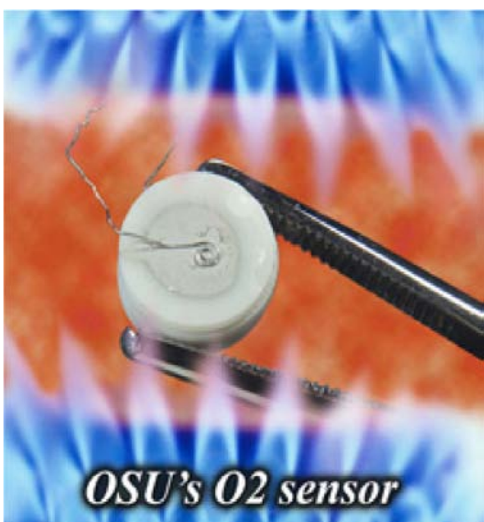
High-Temperature Ceramic Microsensor Development for Combustion Boiler Optimization

CHALLENGE: Sensing in High Temperature Gas Stream

SOLUTION: Ceramic Based Micro Gas Sensors

The Ohio State University's Center for Industrial Sensors and Measurements (CISM) successfully completed a research and development of high temperature ceramic-based microsensor arrays. The purpose of the array is to monitor total concentrations of gaseous nitrogen oxides (NO_x), carbon monoxide (CO), and oxygen (O_2) within the hot zones of the burner (480-815 °C) of a coal-fired boiler and other applications where the environment has high temperature gas.

The research strategy focused on the selection and development of ceramic materials and composites that enabled highly selective sensors for each gas using novel sensing principles that allow for operation at high temperatures in harsh combustion environments. Pattern recognition algorithms were also employed to help extract quantitative information about the gas composition from the collective sensor responses.



The microsensor array comprises a thermal resistive CO sensor and electrochemical potentiometric O_2 and NO_x sensors. Resistance temperature detectors are manufactured from metals whose resistance increases with temperature. Potentiometric sensors use the potential difference between a reference electrode and a working electrode as a signal to measure gas concentration. Microsensors of both types may be made small enough (match head-sized or less) so that their response times are a fraction of a second.

The CO sensor is based on titanium dioxide (TiO_2) and is designed to monitor concentrations of 0 – 1,000 ppm. The researchers are studying catalysts for CO selectivity as well as composite pseudo-noise semiconducting TiO_2 for reducing O_2 cross-sensitivity.

The O_2 sensor can monitor oxygen concentrations from 1 percent to 15 percent. It is based on a closed nickel/nickel monoxide (Ni/NiO) reference electrode with yttria stabilized zirconia (YSZ) as the electrolyte.

The NO_x sensor also measures concentrations of 0 – 1,000 ppm and uses YSZ as the electrolyte with metal oxide sensor electrodes. It includes a catalytic filter that is designed to reduce CO interference as well as allow for measurements of total NO_x.

Each of these sensors has been patented. The O_2 and NO_x sensors have been recognized with R&D 100 awards and licensed for commercialization. Additionally these sensors are being refined, packaged, and tested for aerospace applications.

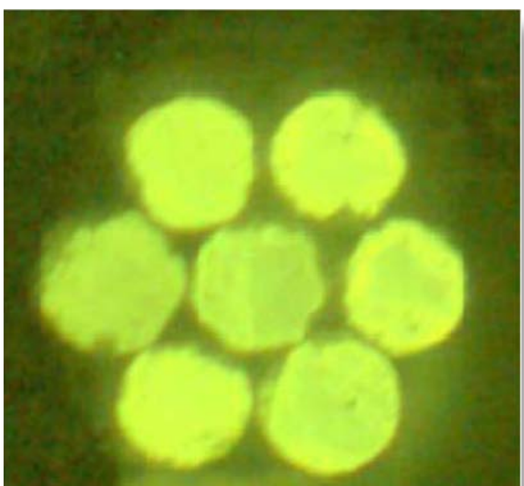
Novel Modified Optical Fibers for High-Temperature in-situ Miniaturized Gas Sensors in Advanced Fossil Energy Systems

CHALLENGE: Advanced Fossil Energy Systems sensors suitable for operation in high temperature, harsh environments

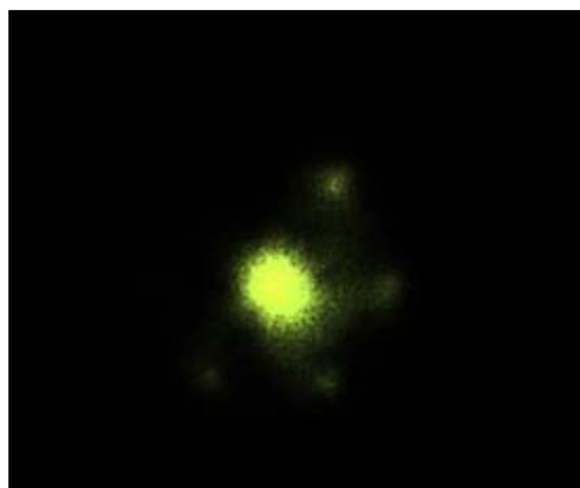
SOLUTION: Develop novel, high temperature gas sensors using modified optical fiber materials

Today's coal-fired power plants and tomorrow's advanced power generation systems will require accurate and reliable gas detection for advanced process control and emissions monitoring . Very few sensors are commercially available for high temperature, harsh environment monitoring of gases—such as nitrogen oxide, sulfur oxide, carbon monoxide, hydrogen, oxygen, methane, and ammonia—which are present in coal and generated in coal-derived syngas applications. Currently available sensors are of limited accuracy, require intensive maintenance, have extremely short lifetimes, and are prone to unexpected failure. The Center for Photonics Technology at Virginia Polytechnic Institute and State University (Virginia Tech), in partnership with the National Energy Technology Laboratory, has worked to develop novel, modified optical fiber materials for high temperature gas sensors based on evanescent wave absorption in standing hole optical fibers.

Virginia Tech was able to demonstrate long wavelength detection by fabricating suitable porous hollow core fibers for use in gas sensors. The research team has produced what is believed to be the first sapphire photonic crystal fiber capable of gas detection in high-temperature, harsh environments. The sapphire photonic crystal fiber was heated to 1600 °C, demonstrating the extremely high temperature capability of these fibers.



Optical micrograph of fiber end-face (reflected light image)



Optical micrograph of the photonic crystal sapphire fiber (transmission mode image)

Micro-Structured Sapphire Fiber Sensors for Simultaneous Measurements of High Temperature and Dynamic Gas Pressure in Harsh Environments

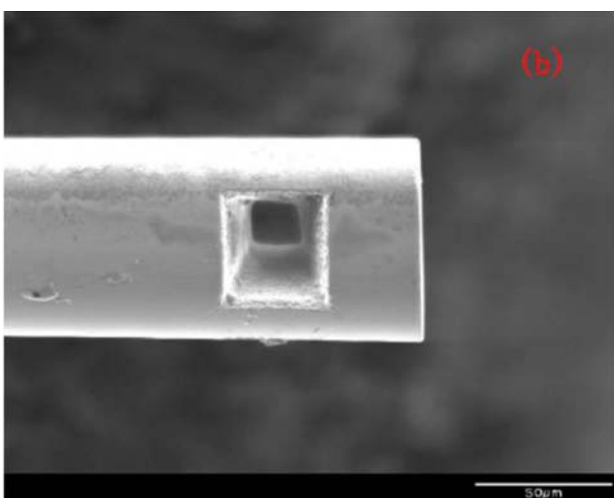
CHALLENGE: Power systems that operate at high temperatures and pressures require more robust sensors

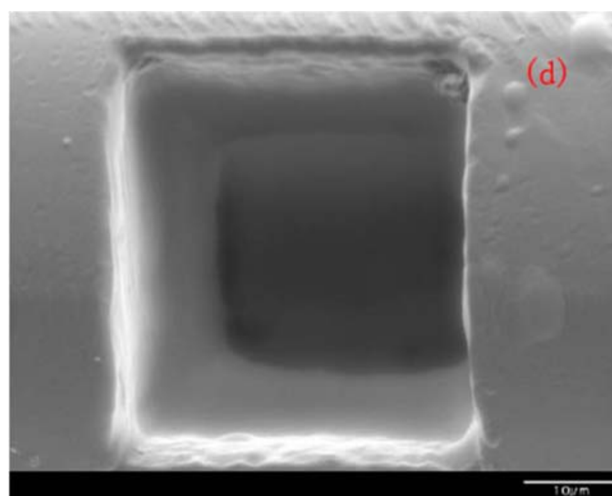
SOLUTION: Develop and demonstrate robust sensors using single-crystal sapphire fibers

Optical fibers are ideal for advanced power system applications that require high-temperature and high-pressure measurements because they are sensitive to the dynamic properties being measured while withstanding harsh environments. This project is developing hybrid extrinsic/intrinsic Fabry-Perot interferometer (HEIFPI) sensors—directly micro-machined on a sapphire fiber using an ultrafast laser—for sensing high temperature and pressure. These hair-thin, cylindrical filaments are made of single-crystal sapphire (glass) able to transmit light by confining it within regions of different optical indices of refraction.

A multidisciplinary research team led by Missouri University of Science and Technology researchers, with members from University of Cincinnati, is working to develop these HEIFPI sensors for deployment in harsh environments. Sensors designed for extreme conditions within gasifiers and turbines will provide valuable data that will improve processes for prediction and prevention of expensive shutdowns and control costly maintenance cycles. Users will implement sapphire sensors into existing fiber optic systems.

Researchers constructed models of the HEIFPI sensors to handle high temperature and pressure. The models were utilized to derive structural parameters of the HEIFPI sensor to guide device fabrication. The team used these parameters to list candidate casing materials and identify the inner and outer layer casing material matrices. The project team has successfully micro-machined the HEIFPI temperature sensor into a hair-like single crystal sapphire fiber that transmits a change in signal due to temperature and heated it to 1,600 °C without breakage. The team is also experimenting with first-of-a-kind cladding materials for encasing the sapphire. Project personnel continue to work on coating sapphire substrates with high-temperature cladding materials and toward commercial application of the HEIFPI sensors.





Scanning Electron Microscope images of HEIFPI sensors (at two different scales) after high temperature treatment.

Integrated Process Engineering and Computational Fluid Dynamics Simulation System

CHALLENGE: Complex and costly design process

SOLUTION: Develop new computational tool

A major success of the AR program is development by NETL of a powerful suite of computational and analytical tools used to model and simulate advanced energy and power generation system processes. Known as the Advanced Process Engineering Co-Simulator (APECS), this innovative software enables engineers to better understand and optimize power plant performance with respect to fluid flow, heat and mass transfer, and chemical reactions.

APECS also has applicability to other process industries such as petroleum, chemicals, and pharmaceuticals. To date, engineers and researchers in more than a dozen organizations worldwide use APECS to address challenges of designing next-generation plants to operate with unprecedented efficiency and near-zero emissions, while operating profitably amid cost fluctuations for raw materials, finished products, and energy.

By coupling computational fluid dynamics (CFD) with advanced visualization and high-performance computing, APECS can be used as a virtual plant simulation tool. Being able to literally view the entire plant or process on multiple, large screens provides developers unique opportunities to try options and immediately view results. Practically, this process will reduce the time, cost, and technical risk of developing high-efficiency, zero-emissions power plants.

The approach used to transfer the APECS software to the private sector includes a DOE-funded cooperative R&D project agreement among NETL; ANSYS/Fluent, the world's leading supplier of CFD software and services; Aspen Technology, a major supplier of process simulation software; Carnegie Mellon University; Iowa State University; West Virginia University; and ALSTOM Power, a major worldwide industrial supplier of power generation equipment and services. The process and energy industries manage some of the most complex and expensive plants in the world, spending nearly $600 billion annually in plant design, operation, and maintenance. The development, transfer, and commercialization of APECS, through NETL's leadership and innovation efforts, are helping these industries to accelerate technology development and reduce associated uncertainties and risks.

NETL researchers conduct a virtual power plant simulation using NETL's APECS tool.

Kinetic Database Coupled to Multiphase Computational Fluid Dynamic Models

CHALLENGE: Availability and implementation of kinetics for computational modeling of fossil energy devices

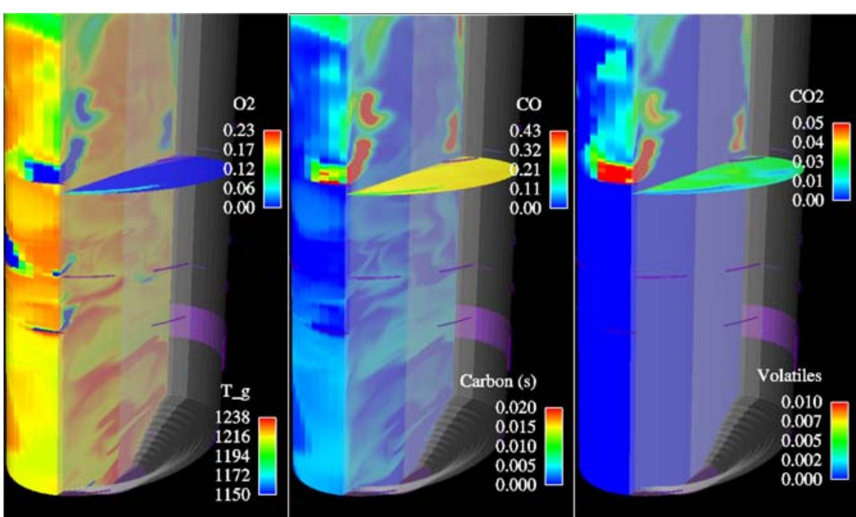
SOLUTION: Develop a kinetic database which interfaces with computational models

A major challenge in modeling reacting multiphase flows encountered in coal combustion, gasification and gas stream pollutant removal such as carbon dioxide capture and sulfur removal is availability and access to kinetic data. Organizing kinetic data in a format that is required by most multiphase computational fluid dynamic (CFD) models is not a trivial task. Availability of kinetic information is scattered across a variety of sources with no easy way to evaluate or compare kinetic information from which one could make an informed decision on the choice of kinetics to use. Recently, researchers from NETL have leveraged the existing software developed under NETL's AR program MFIX (Multiphase Flow with Interphase eXchanges) with NETL's patent pending software C3M (Carbonaceous Chemistry for Computational Modeling). Both pieces of software have received FLC awards and MFIX has recently been recognized for its state-of-the-art technical capability with a 2008 R&D 100 award.

The unique combination of MFIX and C3M has allowed researchers at NETL to develop and validate a model of the Transport Integrated Gasifier (TRIG) in operation at the National Carbon Capture Center in Wilsonville, Alabama. This model was validated using bituminous, sub-bituminous, and lignite coals under air and oxygen blown conditions. Results from MFIX-C3M model are shown in Figure 1. In this figure, the results from chemical reacting MFIX simulation of a commercial scale TRIG unit are shown. Profiles of O_2, CO and CO_2 are shown for a horizontal slice in the vicinity of the coal feed nozzels. These profiles are superimposed on axial fields showing the gas temperature in Kelvin and the mass fractions of carbon and volatiles remaining in the coal as it enters the gasifier.

The model was later used to aid in the commercial scale-up efforts for this technology and the coupling between C3M and MFIX was used to develop an user defined subroutine for the commercial software ANSYS-FLUENT which uses the kinetic information from C3M.

Since the early version of C3M could only handle few coal types, valid for a narrow range of operating condition, funding in part from AR program has been used to expand the range of C3M applicability. The expanded C3M, which is a collaborative work between NETL and West Virginia University, addresses the challenge of incorporating kinetics into a multiphase CFD model from various sources of kinetic information. Under this project the kinetic data base in the original version of C3M has been significantly enhanced by coupling C3M with the commercial software PC Coal Lab and a graphical user interface (GUI) has been developed. PC Coal Lab contains one of the most comprehensive coal kinetic data bases in the world. This new version allows users to conduct MFIX or ANSYS-FLUENT simulations using most any type of coal and account for effects of temperature, heating rate, pressure, and coal particle size on the kinetic rates and yields through the primary and secondary pyrolysis stages. The GUI displays graphs showing the effects of the temperature, heating rate, pressure, and coal particle size on rates and yields for a particular coal or different coals of interest which allows users to quickly asses these effects to determine an appropriate set of kinetics to be incorporated into a MFIX or ANSYS-FLUENT simulation.



MFIX-C3M results from a commercial scale TRIG.

Work under this collaborative project is ongoing with near term goals to continue to expand the C3M operational architecture to include integration with the commercial code Barracuda by CPFD Software and add the kinetic data base CPD (Chemical Percolation Devolatilization) developed at Brigham Young University. In addition, the new data being generated at NETL on coal/biomass mixtures will be included in C3M.

Development and Validation of Multiphase Flow Models for Polydisperse Systems

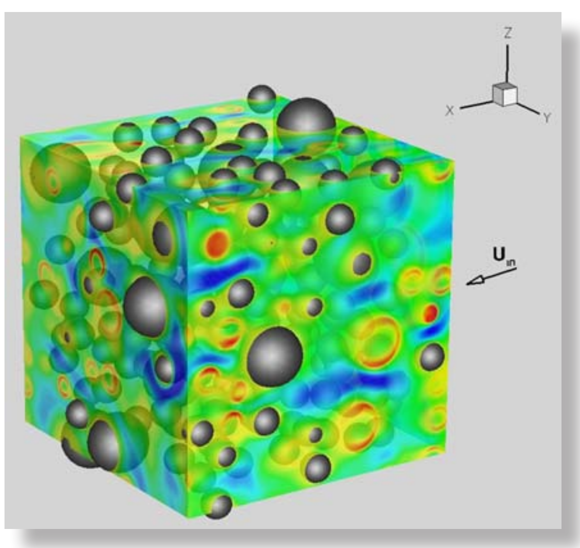
CHALLENGE: Excessive development time and high investment costs associated with the Scale-up of advanced power systems

SOLUTION: CFD Simulator based on first principles

Reactors used for the conversion of coal to energy have traditionally been designed using a build-and-test method, resulting in suboptimal performance in terms of both efficiency and carbon emissions. First-principles models can help to overcome such obstacles, yet their application to practical systems has remained limited due to simplifying assumptions. For example, coal feedstock is characterized by a distribution of particle sizes and such a distribution is known to significantly impact reactor performance, yet most existing models assume identical particles.

In this project, the University of Colorado has teamed with researchers at Iowa State University, NETL, Princeton University, and Particulate Solid Research Inc. (PSRI) to develop fundamental descriptions of polydisperse multiphase flows, including gas-solid interactions, solid-solid interactions, and turbulence. The approach being used involves the bridging of micro-scale effects to macro-scale behavior via simulations ranging from direct numerical simulations (DNS) to continuum models. This multi-scale approach ensures that important physics are retained upon scale-up. The resulting computational fluid dynamics (CFD) model is being validated with a carefully designed set of experiments that cover a range of vessel sizes and operating conditions.

This continuing effort has also been shared with the technical community via nearly 100 presentations and over 30 journal publications to date. The new polydisperse multiphase flow model has been fully incorporated into the award-winning MFIX software suite developed by DOE NETL, which is available to researchers worldwide. These models, as incorporated into MFIX, can be used to critically assessed novel designs prior to the build-and-test phase, thereby greatly reducing the time to market and resource investment. The models and software can also assist in evaluating current designs and problem solving associated with systems that contain multiphase flow compositions.



Direct numerical simulation (DNS) of flow past a bi-disperse suspension of spheres as used to develop polydisperse drag laws.

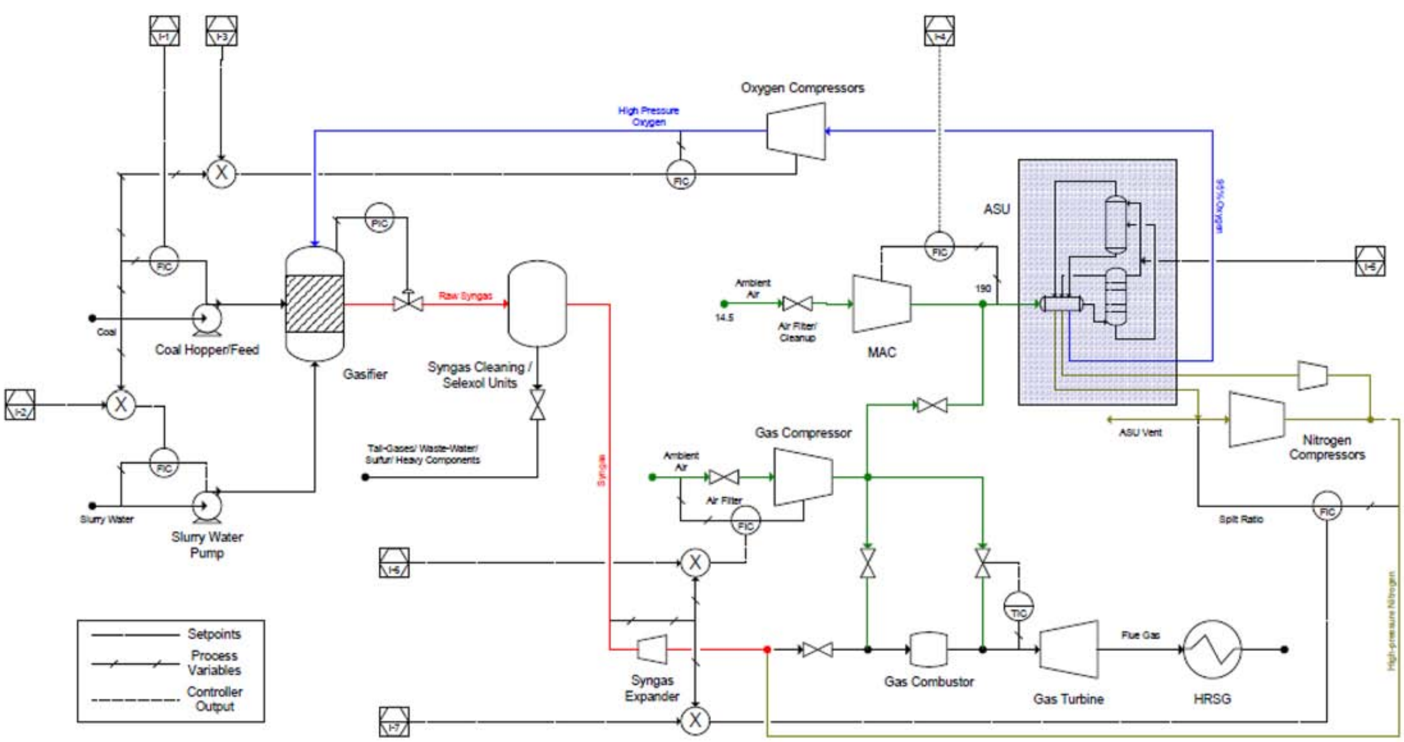
Model Predictive Control of Integrated Gasification Combined Cycle Power Plants

CHALLENGE: Need to better understand how the process design of an integrated gasification combined cycle (IGCC) power plant affects the dynamic operability and controllability of the process

SOLUTION: Develop and test advanced control strategies based on a dynamic simulation model

Integrated Gasification Combined Cycle (IGCC) plants represent one of the most promising options for processing fossil fuels, such as coal or heavy refinery residues, to meet future more stringent environment regulations. IGCC plants need improved process control techniques to operate within constraints, in a safe and optimized fashion. Researchers at Rensselaer Polytechnic Institute are collaborating with researchers at West Virginia University (WVU) to understand how the process design of an IGCC power plant affects the dynamic operability and controllability of the IGCC process.

The researchers developed a dynamic simulation model to predict the process behavior during startup and shutdown, as well as load-following operation, of the IGCC power plant. The model was developed by integrating customized unit models into a dynamic simulation and then confirming the consistency with the steady-state simulation; the resulting pressure-driven model represents a much deeper knowledge of equipment design than was available from previous steady-state designs. Using this dynamic simulation model, the researchers developed model predictive control (MPC) strategies for individual unit operations as well as for the integrated plant. The models and advanced control strategies have enabled researchers to better understand the operability, controllability and various dynamic transients involved in the process, especially during demand fluctuations, and to operate the process in a safe and optimized manner. The project has also contributed to student education in many chemical engineering undergraduate courses, including process design and control, and has helped students understand the challenges of developing clean energy technology to help meet future energy needs, while simultaneously considering environmental constraints.



Aspen flowsheet model developed for analyzing design and control of an IGCC power plant.

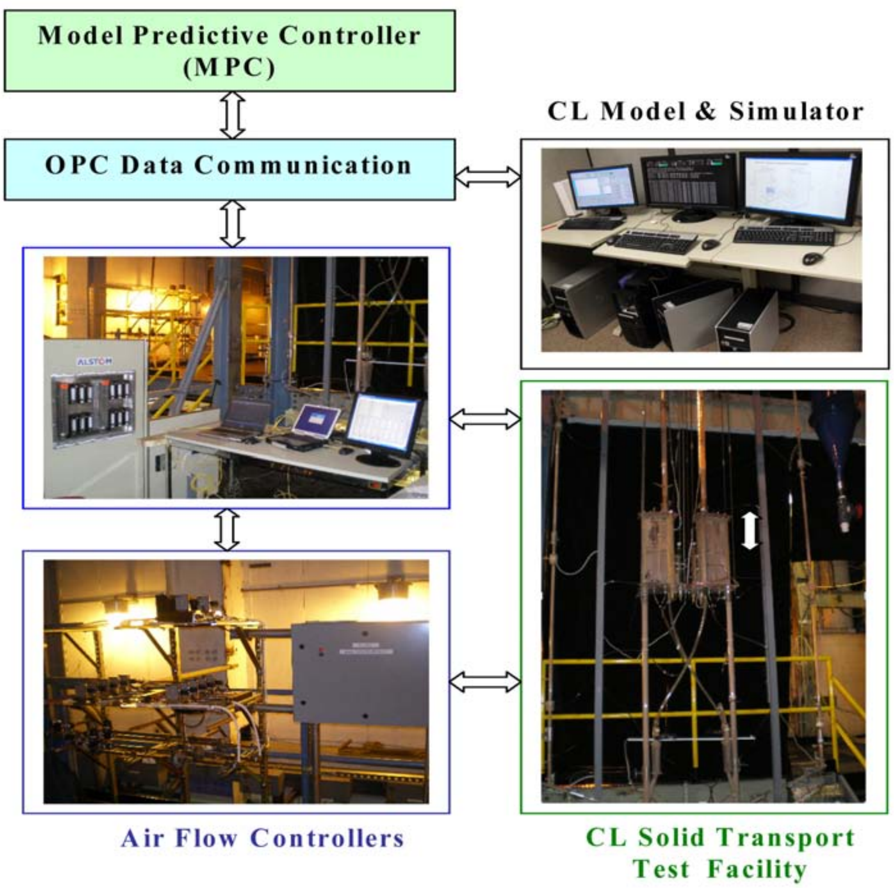
Development of Computational Approaches for Simulation and Advanced Controls for Hybrid Combustion-Gasification Chemical Looping

CHALLENGE: Hybrid Chemical Looping (CL)-based plant improvements with advanced controls

SOLUTION: Develop model-based controls that can be used to operate and better optimize the CL system

Hybrid Chemical Looping (CL) is among the best future alternatives for advanced clean coal power generation in terms of thermal efficiency, potential for high carbon dioxide (CO_2) capture efficiency, and low levelized cost of electricity. It is recognized that high quality process controls (critical for stabilizing multi-loop operations and optimizing performance goals) must be developed to operate this innovative CL system in a safe, integrated, and optimized fashion. Researchers at Alstom Power in Windsor, Connecticut have developed new approaches to model development for simulation and control algorithm development for CL systems.

The researchers applied first principles and pilot-scale experimental data to derive and develop the partial differential equations (PDEs) and nonlinear reduced order models (ROM) needed to simulate the CL process, and have verified the validity of these models against an industry based bench-scale unit. Verification and further model development have enabled researchers to derive a multi-loop mass/momentum/energy balance-oriented set of dynamic process models and integrate it into a real-time dynamic simulation tool to validate and examine transient control cases. Real-time simulation and bench scale testing have shown that this approach is more capable of stable and robust operation than traditional controls alone at operating the dual loop solid transport system.



Conceptual schematic of chemical looping modeling and controls.

Environmentally Safe Control of Zebra and Quagga Mussel Fouling

CHALLENGE: Major power plant water intake fouling by aquatic organisms

SOLUTION: Develop biological control agent

Power plants have been faced with a major problem—zebra and quagga mussels, invasive strains of very small mollusks, have been clogging power plant water intakes since first seen in U.S. waters in 1988. They have colonized many waterways throughout the Missouri-Mississippi-Ohio river basins, from the Canadian border to the lower Mississippi River and toward the northeastern United States. This innovative AR study coordinated with the New York State Museum has shown that a strain of naturally occurring bacteria, *Pseudomonas fluorescens*, is selectively lethal to zebra and quagga mussels, but benign to fish and other bivalves. Experimental treatments have achieved up to 98 percent mussel kill, allowing power plants and other facilities to reduce or eliminate the use of chlorination, reducing the risk of potentially harmful effects of chlorine on aquatic ecosystems.

This research addresses a serious economic and environmental challenge with the development of an innovative biological control solution.

The Pseudomonas fluorescens strain is toxic to zebra mussels, but benign to non-target organisms.

Credits: New York State Museum, D. Wray (inset)

The small zebra mussels densely colonize inside cooling water intake pipes of power plants, thus leading to significant power outages and expense.

Thermal Precombustion Mercury Removal Process for Low-Rank Coal-Fired Power Plants

CHALLENGE: Controlling mercury emissions

SOLUTION: Precombustion mercury removal

Increasingly stringent Federal and State limits on power plant mercury emissions have required innovative emission control solutions. AR teamed with WRI, Alliant Energy, Etaa Energy, Inc., and Montana-Dakota Utilities to develop this unique mercury control technology. This research investigated two-stage thermal pretreatment of raw low-rank coals to remove both moisture and mercury before the fuel goes to a conventional pulverized-coal boiler. Testing has successfully demonstrated that precombustion thermal treatment of coal is a very promising technology, with strong commercial potential. This technology is expected to be able to remove 80 to 90 percent of the mercury cost effectively through the combination of pretreatment reduction and conventional downstream particulate control equipment.

Process Development Unit at WRI Advanced Technology Center provides pilot-scale testing of advanced pollutant removal techniques.

Better Predictions of PAH Bioavailability in Contaminated Sediments

CHALLENGE: Identify hydrocarbon contaminant concentrations

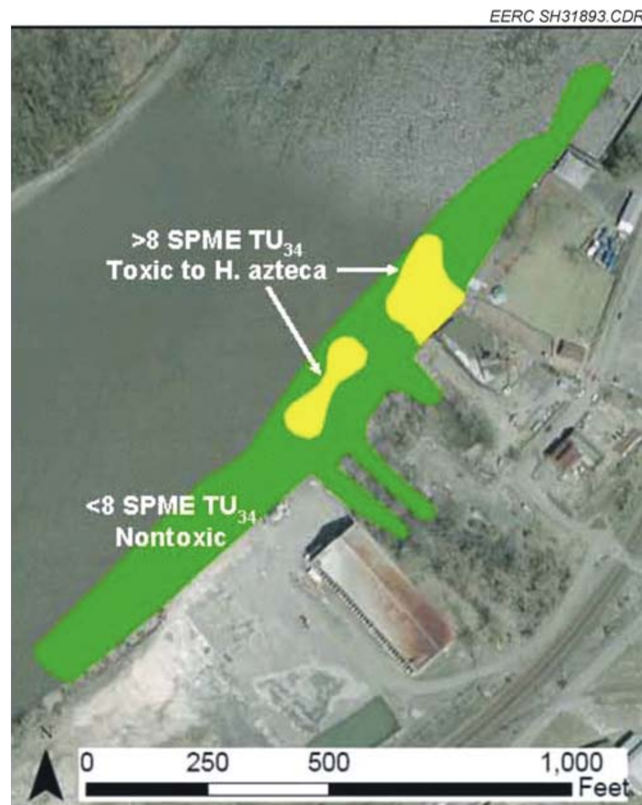
SOLUTION: Develop new analytical technique

The EERC has joined with an industry consortium—the Sediment Contaminant Bioavailability Alliance (SCBA)—and DOE/FE to develop the first suitable analytical method to determine concentrations of polycyclic aromatic hydrocarbons (PAH) in sediment pore water and has applied the method to predict PAH bioavailability. PAHs are chemical contaminants from the burning or degrading of coal, gasoline, fuel oil, and such petroleum-based products as asphalt paving. They accumulate in the benthic, or bottom, sediments of watersheds, and can affect bottom-dwelling organisms such as clams and oysters, potentially causing negative health effects in humans and wildlife.

Current practices regulating PAHs in sediments are based on total concentrations, rather than only those that are bioavailable. However, recent studies have demonstrated that sediment PAH concentrations cannot be used to predict PAH bioavailability and environmental effects, because of the tight binding of PAHs to contaminated sediments. Accordingly, the U.S. Environmental Protection Agency (EPA) proposed measuring PAHs in sediment pore water (the water between the sediment particles) as an improved predictor of sediment PAH effects. However, no analytical method existed that could meet the practical requirements of site surveys.

The EERC method was compared to toxicity tests on the sensitive benthic organism *Hyalella azteca (H. azteca)* on sediment samples from 14 former manufactured gas plants (MGP) and related industrial sites, and found to greatly improve the prediction of PAH bioavailability compared to existing regulatory practices. EERC and the SCBA have successfully moved EERC's SPME pore water analytical technique from R&D status into an active EPA testing protocol, although the corresponding American Society for Testing and Materials (ASTM) protocol remains provisional, pending a multilab round-robin study.

The one-of-a-kind SCBA PAH database continues to add value as a site characterization tool and has direct application in the evaluation of monitored natural recovery as a remedial strategy for sediments. In the sites studied to date, these investigations have demonstrated that remedial actions can be focused on a small fraction of many MGP sites and still full protect human and environmental health. EERC is currently developing analytical methods for evaluating PCB bioavailability and bioaccumulation by macrobenthic organisms, i.e., those large enough to be seen by the naked eye.



Using sediment pore water PAH concentrations to delineate impacts focuses remedial design on areas of toxicity.

WRI Thermal Enhancement (WRITE) Process for Pipeline Ready Heavy Oil

CHALLENGE: Accessing bitumen from tar sands

SOLUTION: Develop new recovery process

Bitumen is an abundant and highly condensed semi-solid form of crude oil. This natural asphalt is an important national resource, but can be hard to recover and refine from tar (oil) sands without using conventional but expensive enhanced recovery methods. AR initiated research with WRI to develop a field upgrading process known as the WRI Thermal Enhancement (WRITE) process. The WRITE Process is helping to make conversion and upgrading of bitumen from Canadian oil sands more economical. Also participating are an industrial partner, MEG Energy Corporation, Calgary, Alberta, which holds options for Canadian rights to the process *and* the site where the process will be piloted; and SNC-Lavalin, a Montreal, Quebec Architect & Engineering (A&E) firm specializing in process and facility design. This process is designed to upgrade bitumen near oil sands production fields, making it unnecessary to add costly diluents prior to transport through pipelines to a central location. Further development and future commercialization of the WRITE process add to the likelihood of successful utilization of this abundant but expensive and difficult-to-extract fossil fuel resource.

Map showing the location of the Athabasca Oil Sands where the WRITE process will be piloted.

Development of Metallic Filters for Hot Gas Cleanup in Pressurized Fluidized Bed Combustion Applications

CHALLENGE: High capital costs of IGCC

SOLUTION: Develop low-cost hot-gas filter

The Inorganic Membrane Technology Laboratory (IMTL) at the Oak Ridge National Laboratory (ORNL) developed a process to manufacture low-cost porous filter media. Through this AR joint technology development project, IMTL succeeded in adapting this exacting manufacturing process to iron aluminide (Fe_3Al) materials using a high-shear gas-atomized powder that was developed and fabricated at Ames Laboratory with assistance from IMTL metallurgists.

Iron aluminide is a corrosion-resistant material that holds strong potential as a long-lasting filter medium in IGCC and other advanced combustion system applications. The filter is used to trap particles from hot synthesis gas *before* those particles can enter and contaminate the gas and steam turbines — which would otherwise reduce efficiency and shorten the lifetime of the turbines.

The aim was to reduce filter cost through design optimization. A separate CRADA with Pall Corporation, a leading manufacturer of filter elements, enabled ORNL to successfully transfer the new technology. Pall added the iron aluminide filter to its S-Series PSS® Filter Element product line, where it has become a best-selling filter with more than 2,000 sales to date.

Photograph of a Pall Corporation iron aluminide hot-gas filter. These filters, made from an ORNL-developed alloy, give excellent performance in coal gasification plants. Over 2,000 are now in use, some for over six years.

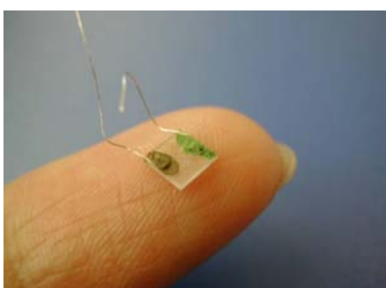
Development and Application of Gas Sensing Technologies to Enable Boiler Balancing and High-Temperature Total NO_x Sensor

PROBLEM: Need durable, effective sensors

SOLUTION: Advanced, compact sensors

A number of AR project efforts are focusing on combustion optimization through improved sensor technology. Integrating such sensors into combustion systems provides emissions reductions accompanied by associated efficiency improvements. To help meet these goals, high-temperature carbon monoxide (CO) and oxygen (O_2) sensors were developed by researchers at The Ohio State University, GE Reuter Stokes, and other participants from industry and academia, with funding from NETL, as part of a broad effort to more closely monitor total nitrogen oxides (NO_x), CO, CO_2, and O_2 during combustion. Both the CO and O_2 sensors received R&D 100 awards by an independent judging panel and the editors of *R&D Magazine* in 2005, as being among the 100 most technologically significant products introduced into the marketplace over the previous year.

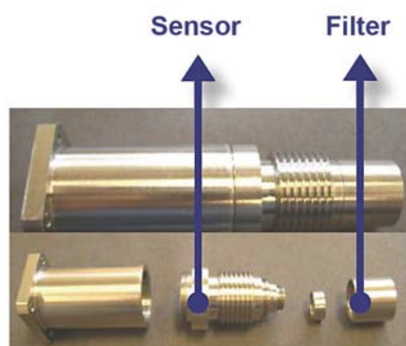
The O_2 sensor is very small and does not require an expensive external O_2 reference, relying instead on an internal metal/metal oxide reference sealed by a unique deformation bonding method to generate a fixed partial O_2 pressure. The sensor is fabricated from relatively common and inexpensive ceramic materials that can withstand the environment inside a combustion chamber. These features enable multiple O_2 sensors to be placed throughout a combustor, allowing the operator to map the combustion process and control it more tightly, leading to higher efficiency and lower emissions.



High-temperature Total NO_x Sensor is highly miniaturized and resistant to harsh combustion conditions.

As an additional payoff from this research, the underlying technology for a high-temperature total NO_x ($NO + NO_2$) sensor has been developed and patented by Ohio State with support from NETL's AR program. The central feature of the NO_x sensor is a platinum-based porous catalyst filter that filters out elements that otherwise would skew measurements. This filter also eliminates the need for an additional air reference sensor. The high-temperature total NO_x sensor was selected for an R&D 100 award in July 2007 by an independent judging panel and the editors of *R&D Magazine*. The sensor exhibits parts-per-billion (ppb) sensitivity, is capable of operating at temperatures as high as 700 °C, and is resistant to interference from common gases in the combustion stream, such as CO, CO_2, hydrocarbons, ammonia, and water. In addition, integration with a platinum-based sensing element has led to miniaturization of the sensor. These characteristics enable use of these sensors in low-NO_x combustion processes such as in power generation with turbines, in diesel engines for trucks and passenger vehicles, and even, most recently, in breath analysis for asthma patients.

EmiSense, a recent spin-off company from Ceramatec Inc., has licensed exclusive patents from Ohio State for the sensor, which is being marketed as NO_x Trac™. Ceramatec is a 30-year old technology incubator whose business strategy involves spinning off successful new companies, such as EmiSense, when high-potential technologies become commercially ready. The National Science Foundation (NSF) and the Glenn Research Center of NASA have provided additional funding for aspects of Ohio State's microsensor research.



A typical filter package is shown above housing the filter and sensor.

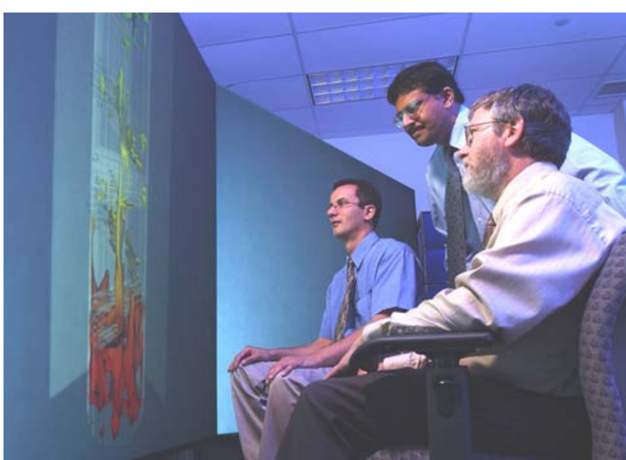
Multiphase Flow with Interphase eXchanges (MFIX)

CHALLENGE: Expensive power plant scale-up

SOLUTION: Simulates plant performance

Developing the technologies needed to use coal cleanly, efficiently, and with less carbon emissions entails repeatedly building and testing designs at several different scales. This build-and-test method increases the cost of developing new technologies, which limits engineers' abilities to develop the novel designs that are needed to achieve near-zero emissions in future power plants. A much-needed software suite known as "MFIX" has been developed at NETL with support from Aeolus Research, Inc. (Dunbar, PA.), Parsons, Inc. (Morgantown, WV), and ORNL. MFIX reduces the cost of developing and commercializing advanced coal technologies through intricate simulations.

Developed over many years with support from AR's Computational Energy Sciences, MFIX solves physics-based equations to simulate high-solids-loading flows that occur in critical equipment items, such as coal gasifiers, allowing engineers to replace expensive build-and-test steps with much cheaper simulations, thereby encouraging the discovery of radically novel designs. MFIX is being used by researchers around the world to model a variety of processes ranging from coal gasification to volcanic eruption flows. In 2006, MFIX won an award for Excellence in Technology Transfer from the Federal Laboratory Consortium (FLC), while in 2007, MFIX received a prestigious R&D 100 award for technological excellence from *R&D Magazine*.



Using MFIX, NETL researchers study a visualization of a power plant component.

Sorbent Enhancement Additives for Mercury Control

CHALLENGE: Remove mercury from combustion of low-rank coals

SOLUTION: Improve activated carbon reactivity by sorbent enhancement

Because gaseous mercury can be present as either oxidized or elemental mercury, any effective control strategy must optimize control of both. Plants firing lower-rank coals, including subbituminous and lignite, are considered to have the most problematic and/or challenging mercury capture applications because these coals have low chlorine content, resulting in mercury emissions that are mostly elemental, thereby making capture more difficult.

Early tests by the EERC showed that activated carbon injection (ACI) was somewhat effective at capturing mercury from combustion of these coals but was, in most cases, limited to about 60 percent removal, regardless of how much AC was injected. Several projects using subbituminous and lignite coals showed less than 50 percent removal using standard ACI, even at high injection rates whose levels were considered uneconomical and unacceptable by most utilities.

To overcome this limitation, the EERC developed a sorbent enhancement additive (SEA) technology that significantly improves the reactivity of AC, thereby making it much more effective at capturing both elemental and oxidized forms of mercury. The technology can also improve native capture by existing fly ash and can improve oxidation for subsequent removal by downstream sulfur dioxide (SO_2) control systems.

Antelope Valley Station, near Beulah, ND.

Through successful testing at many power plant test sites, the SEA technology has consistently shown that significantly less AC can be used when combined with SEAs, providing better economics and fewer potential balance-of-plant impacts. In most cases, the amount of AC can be decreased by a factor of 2–4, yet provide higher levels of mercury capture. The SEAs are abundant and affordable, resulting in improved economics as compared to using high injection rates of AC or commercially available treated carbons. Adaptable as well to other industries such as cement production, the SEA technology is available commercially.

Impacts of Lignite Properties on Powerspan's NO_x Oxidation System

CHALLENGE: Simultaneous removal of pollutants from flue gas

SOLUTION: Innovative electro-catalytic oxidation technology

The EERC led a team that involved several industry partners in evaluating air pollution control options as part of the planning process for a new power generating unit at Minnkota's Milton R. Young Station near Center, North Dakota. One technology evaluated was Powerspan's multipollutant control process, called Electro-Catalytic Oxidation (ECO®). The ECO technology is designed to simultaneously remove nitrogen oxide compounds (NO_x), sulfur dioxide (SO_2), fine particulate matter ($PM_{2.5}$), acid gases—such as hydrogen fluoride (HF), hydrochloric acid (HCl), and sulfur trioxide (SO_3)—mercury (Hg), and other metals from the flue gases of coal-fired power plants.

The EERC and its commercial partners designed and fabricated an ECO slipstream reactor system to test the *in-situ* impacts on the electrodes of flue gas derived from high-sodium lignite coal. The core of the ECO technology is a dielectric barrier discharge (DBD) reactor composed of cylindrical quartz electrodes residing in metal tubes. Electrical discharge through the flue gas, passing between the electrode and the tube, produces reactive O and OH radicals that react with flue gas components to oxidize NO to NO_2 and HNO_3, and a small portion of the SO_2 to SO_3 and sulfuric acid (H_2SO_4). The oxidized compounds are subsequently removed in a downstream scrubber and wet ESP.

The reactor was in operation for four months downstream of the ESP on an existing unit at Milton R. Young Station. Following the test period, examination of the electrodes using scanning electron microscopy (SEM) x-ray microanalysis showed significant accumulations of ash coatings rich in sodium, sulfur, calcium, potassium, and silica on the surface of the electrodes. Sodium and sulfur were found to be the main problems in the fouling of the electrodes.

Based on these results, it appears that the ECO technology has potential for new power plant designs that burn high-sodium lignites but are significantly impacted by the sodium-rich ash. Sodium reduction upstream of the reactor and aggressive ECO reactor-cleaning are possible methods that will enable the ECO technology to be feasible. Future testing must be aimed at measures to reduce the sodium aerosol content of the flue gas in order to prevent the formation of sodium-rich deposits.

EERC ST31931.CDR

Inside the Powerspan ECO slipstream reactor.

Conclusion

All of the successes described in these pages, stimulated by NETL's Advanced Research program, have been achieved in concert with many partners—from academia, industry, and other governmental organizations. NETL's own in-house facilities and depth of expertise are augmented by the nationwide reach and specialized talents and resources of other participating organizations. Together, program participants explore the "grand challenges" of fossil fuel research, focusing on breakthrough technologies or novel applications, in the areas of High-Performance Materials, Coal Utilization Science, Sensors and Controls Innovations, Computational Energy Sciences, and other promising approaches such as biotechnology and bioprocessing, pollutant formation and removal, and emissions reduction.

Future AR programs and successes will continue with such collaborations, emerging through innovative projects that pave the way to enhancing our national energy security and energy diversity by improving utilization of the nation's abundant fossil energy resources. These projects are aimed at providing measurable benefits to coal and power systems technologies—improved efficiencies, lower costs, new materials, and new processes. They are designed to create momentum that launches a technology or process on the path from its first, fostering steps in the laboratory through the many stages necessary to achieve the confident stride of full commercial viability.

More information on many of the programs, projects, and technologies described in this brochure—including fuller descriptions of individual project successes as well as project and program fact sheets—may be found on the AR "reference shelf" at the following location on the NETL website: http://www.netl.doe.gov/technologies/coalpower/advresearch/ref-shelf.html

For More Information on Advanced Research Visit:

www.netl.doe.gov/AR

NETL

National Energy Technology Laboratory

1450 Queen Avenue SW
Albany, OR 97321-2198
541-967-5892

2175 University Avenue South, Suite 201
Fairbanks, AK 99709
907-452-2559

3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4764

626 Cochrans Mill Road
P.O. Box 10940
Pittsburgh, PA 15236-0940
412-386-4687

13135 Dairy Ashford, Suite 300
Sugarland, TX 77478
281-494-2516

Visit the NETL website at:
www.netl.doe.gov

Customer Service:
1-800-553-7681

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Contact

Robert R. Romanosky
Technology Manager, Advanced Research
National Energy Technology Laboratory
3610 Collins Ferry Road
P.O. Box 880
Morgantown, WV 26507-0880
304-285-4721
robert.romanosky@netl.doe.gov