NETL-RUA
Regional University Alliance

Shared Laboratories,
Shared Intellect,
Shared Resources

the ENERGY lab

NATIONAL ENERGY TECHNOLOGY LABORATORY

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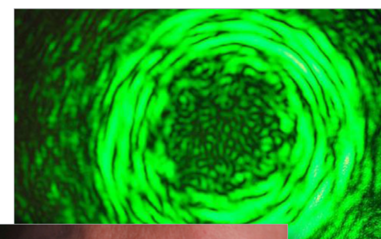
NETL-RUA: Collaborative R&D for Technology Innovation

The U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) has a 100-year history of partnering with academia and industry to solve the nation's energy issues by developing and commercializing new technologies. NETL is continuing these long-standing partnerships through the NETL-Regional University Alliance (NETL-RUA). This partnership combines the facilities, expertise, and resources of NETL with those of five world-renowned research universities—Carnegie Mellon University, the Pennsylvania State University, the University of Pittsburgh, Virginia Polytechnic Institute and State University, and West Virginia University—as well as industry partner URS Corporation, one of the nation's largest and most comprehensive engineering services firms.



NETL-RUA researchers jointly develop and deploy the technologies that enable domestic coal, natural gas, and oil to power our nation's homes, industries, businesses, and transportation while protecting our environment and enhancing our energy independence. In addition to advancing today's technology, NETL-RUA draws on the power of its combined capabilities and experience to create the innovations that will facilitate the transition to a low-carbon energy future.

A keystone of NETL-RUA is its ability to combine experimentation and computational modeling to rapidly screen potential concepts and optimize system performance, resulting in accelerated commercial deployment and creation of new manufacturing and industry jobs. NETL-RUA mentors young professionals by engaging them in its pioneering research and prepares them to be the future leaders of a high-tech energy marketplace.

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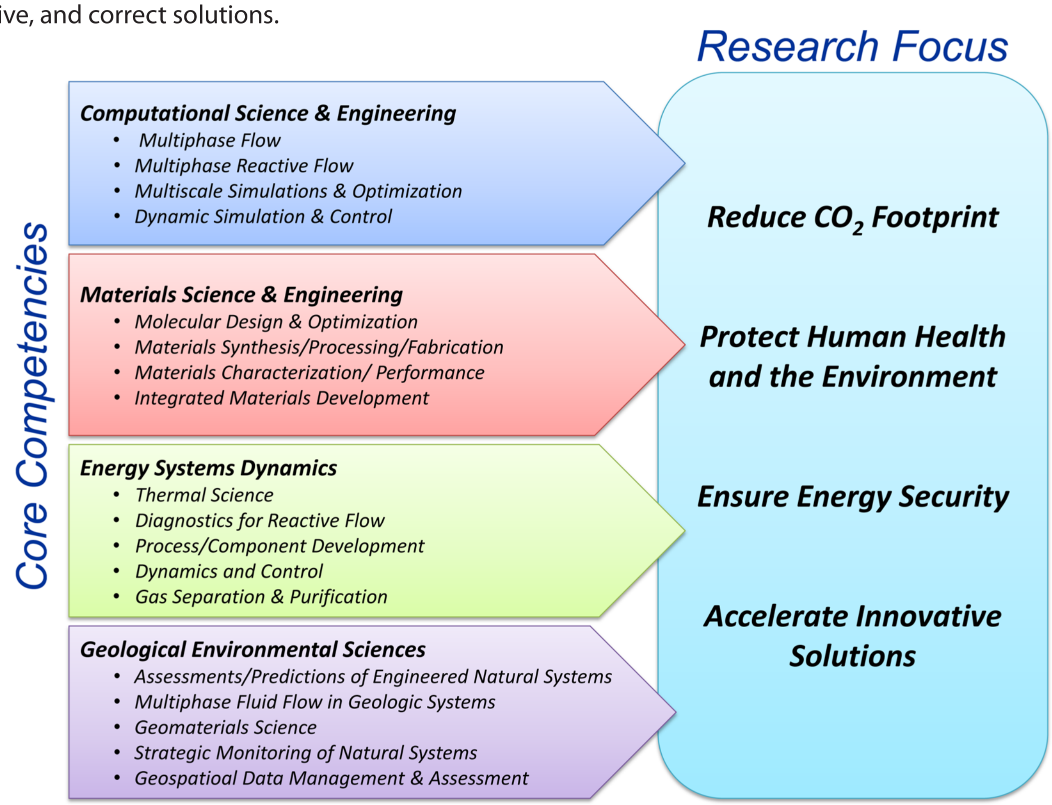
Website: www.netl.doe.gov   Customer Service: 1-800-553-7681

Research Focused on Solutions

NETL-RUA capabilities are focused on solving the nation's most challenging energy issues. Through existing competencies, NETL-RUA can assemble the right team using the right technology to achieve timely, cost effective, and correct solutions.



Reducing the CO_2 Footprint

Reducing carbon emissions from fossil-fueled power plants can be accomplished through various options including optimized designs to improve process efficiency, reduce cost of CO_2 separation and capture, and utilize CO_2. To accomplish this, NETL-RUA researchers are developing high performance materials for system components; highly selective, lower-cost sorbents, solvents, and membranes; and novel CO_2 conversion processes.

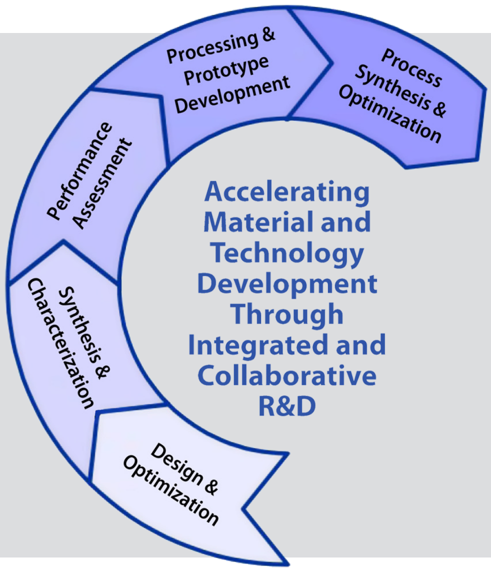
Continued use of fossil fuels is dependent on the ability to safely and permanently store CO_2 over long periods of time. NETL-RUA research efforts are increasing our understanding of CO_2 storage technology including CO_2 migration, revealing potential issues, providing remedies for leakage, and finding more accurate estimates of long-term storage potential.

Protecting Human Health and the Environment

NETL has been instrumental in developing technologies that reduce emissions of sulfur, NOx, and particulate matter. Increasingly stringent emission regulations for fossil-based electric power generation and improved process control require the ability to quickly and cost-effectively measure gas composition and trace contaminants.

Ensuring Energy Security

The safe and clean production of affordable, domestic unconventional fossil energy resources can reduce our dependence on foreign sources of fuel. NETL-RUA research efforts have improved our ability to understand the behavior of these systems and the impacts and issues associated with production of these resources. Efforts also focus on innovative energy systems that will facilitate the transition from a fossil-based energy sector to a sustainable future energy market.



Accelerating Development and Deployment of Energy Technology

Combining experimentation and computational modeling makes it possible to accelerate technology development and deployment by more rapidly screening potential concepts, optimizing system performance, eliminating some scale-up design and testing, and ultimately reducing the risk of commercial deployment. Computer simulations and models can also be used as training tools for the operation and maintenance of advanced energy plants.

Research Recognition & Impact

A good measure of the impact of NETL-RUA research efforts is the number and breadth of awards garnered from outside organizations that objectively compare NETL-RUA research against that of peer organizations and researchers. The Alliance has garnered as many, or in some cases, more awards than other much larger national laboratories.

By that measure, NETL-RUA can be proud of its recognition as a research and technology innovator where "energy challenges converge and energy solutions emerge." Some of the recent awards received by NETL-RUA include:

- Fourteen R&D 100 awards over the past five years
- 2011 and 2012 DOE Secretarial Honor Awards
- 2012 Presidential Early Career Award for Scientists and Engineers
- 2011 International Student Paper contest sponsored by the American Society for Metals International
- Great Minds in STEM™ Hispanic Engineer National Achievement Awards Corporation (HENAAC) award for Outstanding Technical Achievement.
- 2012 Council for Chemical Research Award

NETL-RUA is also home to prestigious researchers who are:

- National Academy of Science Energy Ambassadors
- Fulbright Scholars
- National Academy of Science Fellows

John Kitchin, CMU chemical engineering professor and NETL-RUA researcher accepts the 2012 Presidential Early Career Award for Scientists & Engineers.

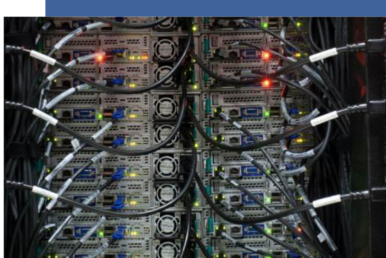
Paul Turner of NETL accepts the 2012 DOE Secretarial Honor Award from Energy Secretary Steven Chu for the team that developed a platinum-chromium alloy that revolutionized heart stent functionality.

RESEARCH SPOTLIGHT

In collaboration with Boston Scientific Corporation, NETL developed a novel platinum-chromium alloy for coronary stent applications. The revolutionary alloy allows for detection by x-ray devices while providing unprecedented flexibility and corrosion resistance. The technology has become the leading stent platform in the world accounting for more than $4 billion in sales since its introduction in 2010.

In collaboration with industry and academic partners, NETL validated and advanced its novel high-temperature, chemically stable catalyst for converting heavy hydrocarbons into hydrogen-rich synthesis gas for use in solid oxide fuel cells. This technology was licensed to start-up company Pyrochem Catalyst Corporation and is under development for commercial applications.

NETL-RUA's Simulation Based User Center's High Performance Cluster, which ranks 54th in the world for speed and scale, is the home to the Carbon Capture Simulation Initiative (CCSI) toolset. The CCSI Toolset provides new models and computational capabilities that will accelerate the commercial development of carbon capture technologies and a broad range of technology development in power, refining, chemicals production, gas production, and more.



Partnership Arrangements

NETL has several different types of partnership agreements that give industrial collaborators unparalleled access to NETL-RUA members and facilities. These include Cooperative Research and Development Agreements, Contributed Funds Agreements, and Nondisclosure Agreements. These instruments enable industrial partners to negotiate agreements that suit their needs including agreements with Go/No-Go decision points to ensure that progress aligns with expectations. Once a technology is developed, it could be available for licensing.

NETL-RUA provides the framework, commitment, and integration of regional capabilities needed to meet the demand for clean, affordable, and abundant energy and secure our nation's energy independence and security.

More information about working with the NETL-RUA can be found at:

www.netl.doe.gov/rua

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RELEVANT LINKS

NETL Annual Review

http://www.netl.doe.gov/rua/about/NETL-RUA-Annual-Review-2011.pdf

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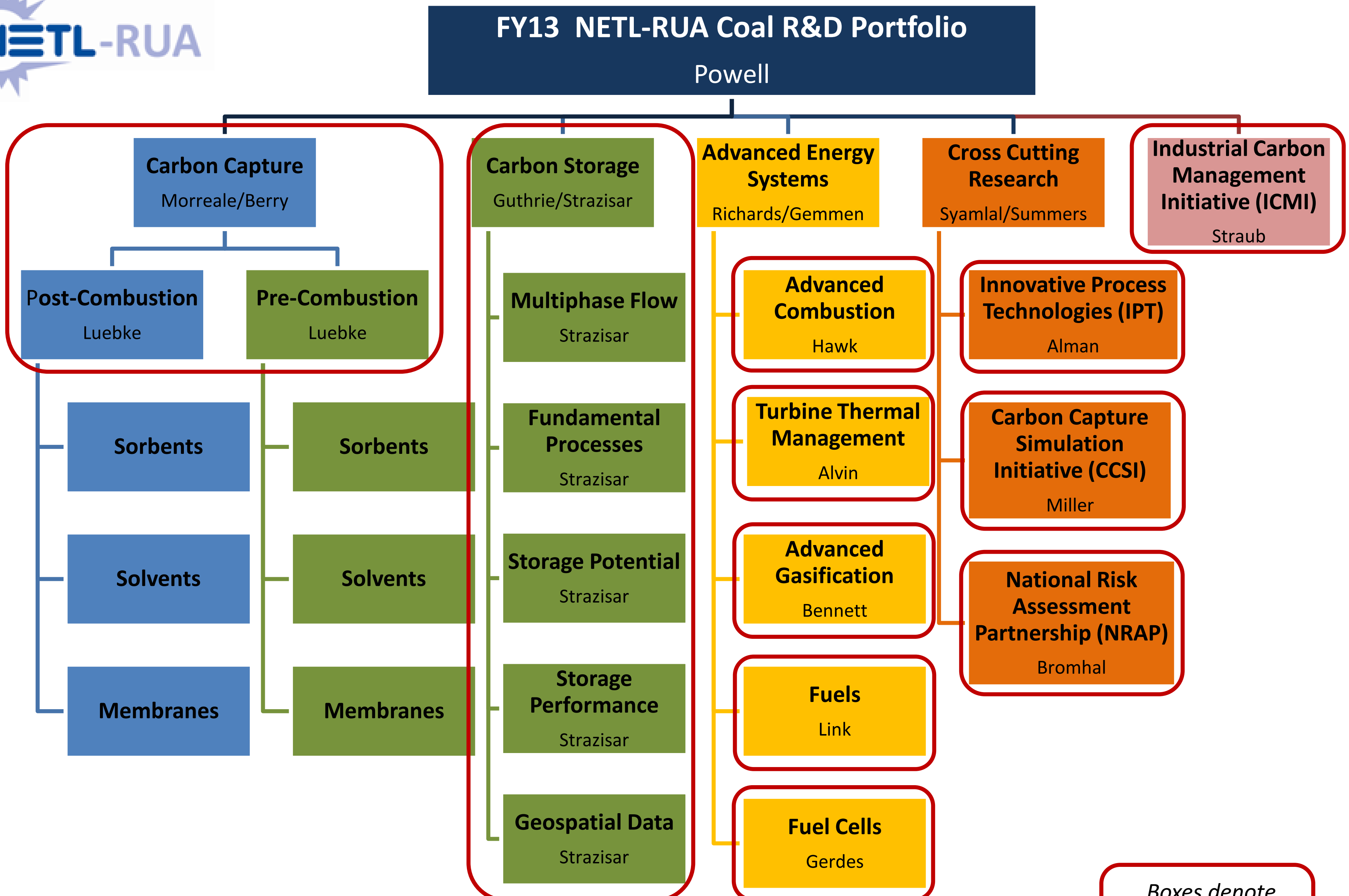
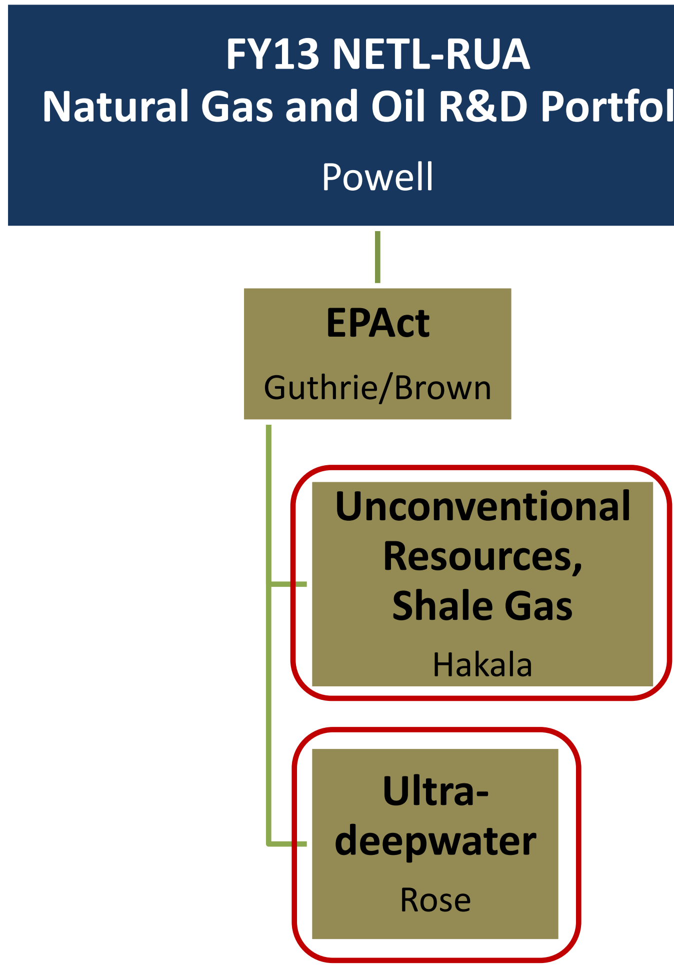


Boxes denote 11 coal R&D research teams

FY 2013 R&D Portfolio: Strategic Center for Coal

Research team fact sheets follow in alphabetical order



Boxes denote 2 natural gas and oil R&D research teams

FY 2013 R&D Portfolio: Strategic Center for Natural Gas & Oil

Research team fact sheets follow in alphabetical order

the ENERGY lab

R&D FACTS

Advanced Energy Systems

Advanced Combustion

Background

Conventional coal-fired power plants utilize steam turbines to generate electricity, which operate at efficiencies of 35–37 percent. Operation at higher temperatures and pressures can lead to higher efficiencies, resulting in reduced fuel consumption and lower greenhouse gas emissions. Higher efficiency also reduces CO_2 production for the same amount of energy produced, thereby facilitating a reduction in greenhouse gas emissions. When combined, oxy-combustion comes with an efficiency hit, so it will actually increase the amount of CO_2 to be captured. But without so much N_2 in the flue gas, it will be easier and perhaps more efficient to capture, utilize and sequester.

NETL's Advanced Combustion Project and members of the NETL-Regional University Alliance (NETL-RUA) will conduct laboratory-scale through pilot-scale tests of advanced oxy-combustion capture technologies that show, through engineering and systems analysis studies, continued achievement toward the goal of 90 percent CO_2 capture at no more than a 35 percent increase in electricity cost.

Advanced Combustion Research at NETL

Experience with steam boilers has provided information on existing boiler alloys, but limited data is available at higher pressure and temperatures. The Advanced Combustion Project addresses fundamental issues of fire-side and steam-side corrosion in oxy-fuel combustion environments. NETL's advanced ultra-supercritical (A-USC) steam autoclave provides a unique capability to examine long-term steam oxidation as a function of pressure, including A-USC conditions.

Oxy-combustion Environment Characterization

Laboratory and field testing will address fire-side corrosion issues during oxy-fuel combustion with emphasis on design considerations, such as flue gas recycle paths and the use of staged combustion burners. In order to better understand the effect of geometry of the laboratory specimen on scale morphology and exfoliation behavior, research will be pursued on the effects of oxide scale constraints (i.e., comparing tube sections with flats), atmospheres (steam, moist air, dry air), and pressure. Scale morphologies from the lab tests will be compared with utility exposures to assess the importance of each test variable for acceptance of laboratory data in scale exfoliation models with time spent on understanding the variation that exists between the two approaches.

Results of this work will provide information on the performance of materials in oxy-fuel combustion environments, which is necessary to select the most cost effective materials for boilers and steam turbines. Research on steam-side corrosion addresses the effect of pressure on steam oxidation in A-USC conditions for test

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URS Corporation

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alloys and determines the role of each oxidant in mixed-oxidant conditions. Evaluating the effect of pressure on steam oxidation is important because this aspect is poorly understood for existing boiler alloys and there is no industrial experience for existing alloys in A-USC steam. For exposure tests with ash covering, analysis of the specimens showed, for example, that boiler alloy T91 had more section loss in the high water flue gas de-sulfurized condition (FGD) with 20% H_2O and without FGD cases. The scale morphologies were 3-layer structures of Fe-Cr-O-S near the metal, Fe-Cr-O in the middle, and a thin Fe-O layer near the ash (see Fig. 1).

Alloy Modeling

In the alloy modeling activity, microstructure characterization has been undertaken on the advanced materials used in USC and A-USC steam power plants. Characterization of these alloys will facilitate physics-based life models, leading to maximum utilization of these materials in power plants. Use of these materials will facilitate cost savings, increase plant efficiency, and reduce CO_2 output.

An experimental protocol for characterizing fine carbides and dislocations within the interior of martensite laths was developed at Virginia Tech in support of this task activity. This protocol utilized transmission electron microscopy (TEM), in particular parallel beam nano-probe electron diffraction and advanced electron tomography. These techniques were used to characterize coarse lath boundary carbides. The result of lath boundary carbide characterization can be summarized as follows:

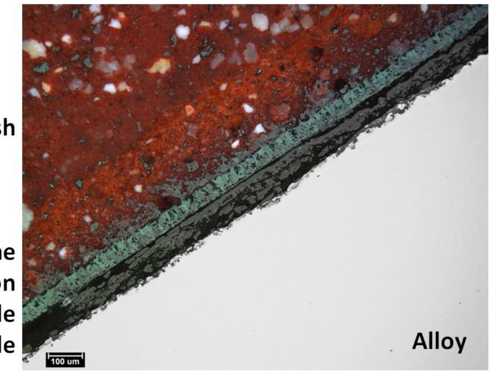

Figure 1. Commercial boiler tube alloy T91 after exposure at 700°C for 240 hours in Oxy, FGD with 20% H_2O

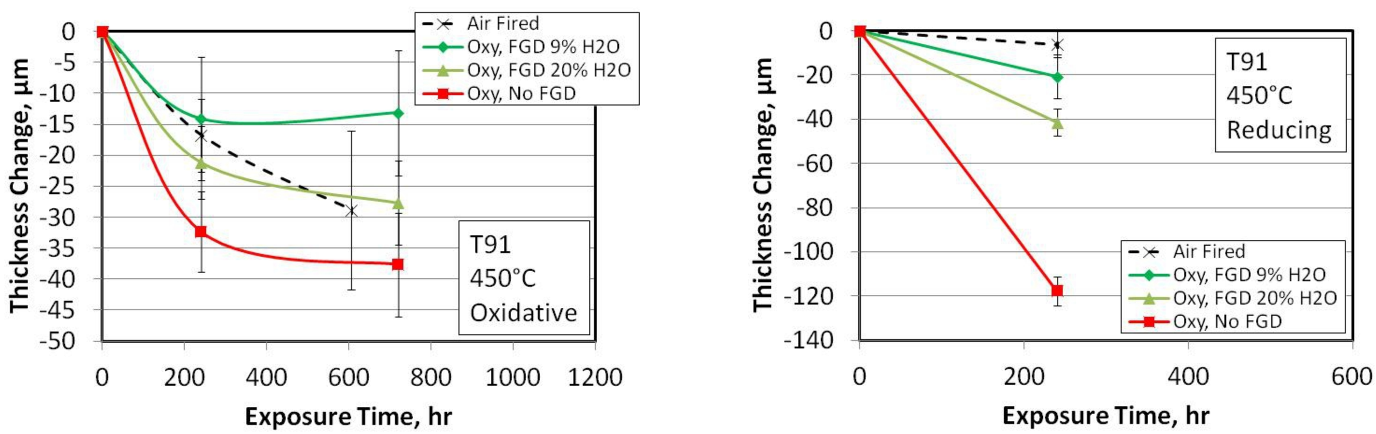

Figure 2: Metal loss for T91 exposed at 450°C in oxidative (left) and reducing (right) atmospheres with thick ash cover, simulating air-fired and three (3) oxy-fired waterwall conditions.

- Determined 2D characteristics of coarse lath boundary carbides. The basic structure of the lath boundary carbides was designated as $Cr_{23}C_6$;
- Used electron tomography (3D mapping) to characterize coarse lath boundary carbides, determining relative orientation to lath as well as length, width, and thickness of carbides;
- Used the 3D precipitate distribution data to assess systematic TEM projection errors in 2D data; and
- Compared data from precipitates in as-received [sample-1] and creep-tested [samples-2] using 3D mapping.

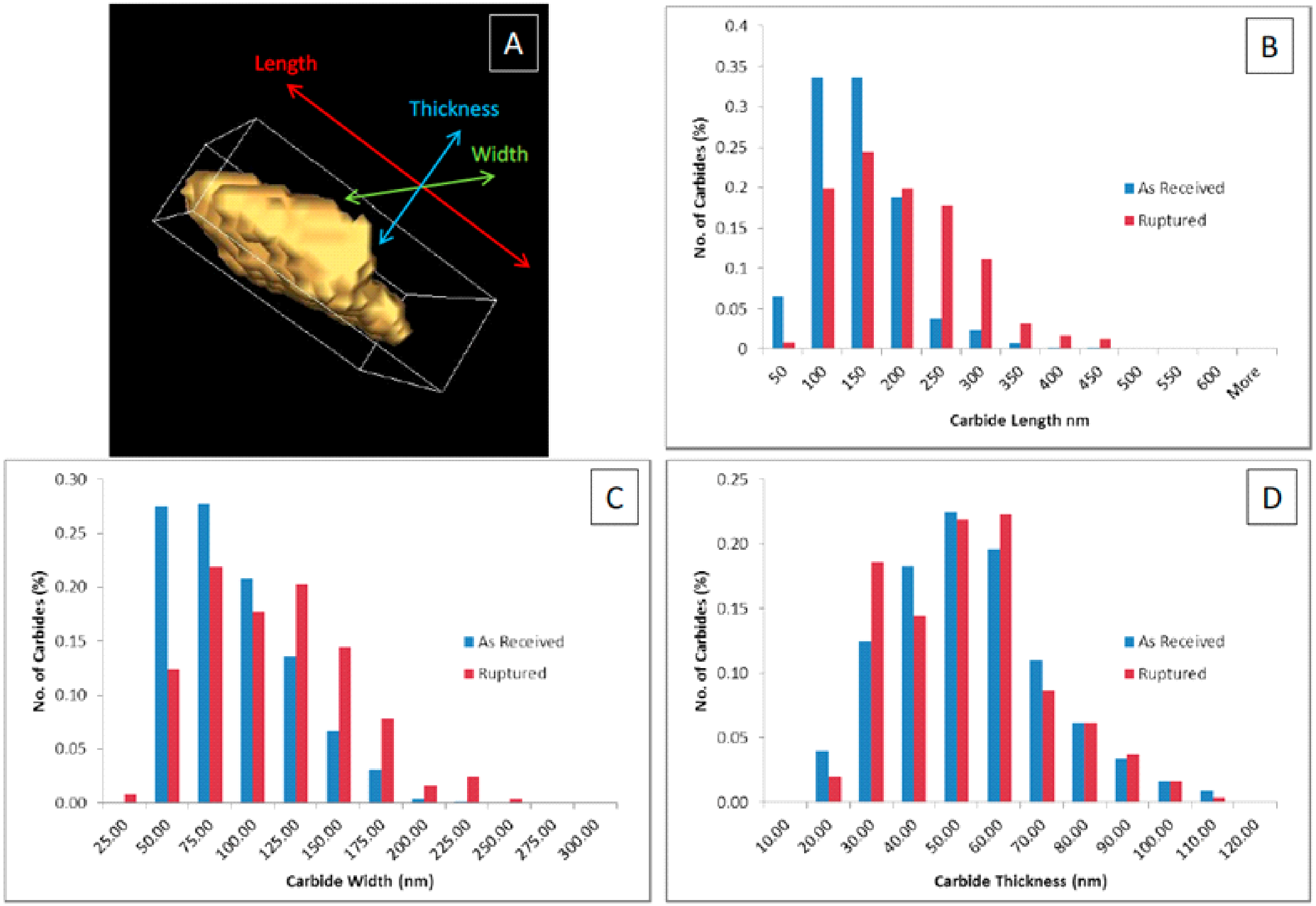

Figure 3: (A) An illustration showing how the dimension of each $M_{23}C_6$ was labeled. Comparisons between as received [sample-1] and creep tested [sample-2] are shown for (B) length, (C) width, and (D) thickness.

Alloy Manufacturing and Process Development

Research is aimed at designing alloys and developing manufacturing processes that can be practically and economically utilized to produce full-scale components for deployment. Work in alloy design and large-scale castings and forgings will focus on alloy design to produce Ni-based castings and steel forgings. Collaboration with industry partners has been pursued to facilitate the supply and process development of large-scale Ni-based superalloy castings for power plant applications.

NETL has developed a unique computational heat treatment approach based on the dendrite arm spacing distance in a casting that allows for a desired degree of homogenization in that particular casting. This heat treatment step individualized for the specific casting of interest and facilitates full development of cast article mechanical strength, especially if strengthened with a second phase like γ′ in precipitation strengthened nickel superalloys. Consequently, a range of castings have been homogenized as indicated using this approach.

- NETL Small Ingots (15#): 1100°C/3 h + 1200°C/9 h
- Metaltek Step Block (300#): 1130°C/3 h + 1200°C/3 h + 1210°C/14 h
- Flowserve Step Block (1000#): 1100°C/6 h + 1200°C/48 h
- Special Metals ESR/VAR (10,000#): 1133°C/4 h + 1190°C/8 h + 1223°C/30 h

NETL has also been working on 9-12% Cr martensitic steels, attempting to develop new alloys with creep life better than existing commercial alloys. Research to date has led to CPJ-7, a martensitic steel that could be used for steam turbine components.

Table 1: Creep life (hours) for CPJ-7 steel tested at 650°C compared to commercial COST steels at selected stress levels.

Alloy/Stress	COST E	COST FB2	COST B2	CPJ-7
25.0	223	614	655	1,454
22.5	---	1,127	---	2,344
20.0	843	1,783	2,428#	5,388
18.0	3,198*	3,483	4,148	12,272
15.0	---	---	---	12,584^

** COST E specimens (avg. of 3 tests) at 16.2 ksi*
 # COST B2 specimens (avg. of 2 tests)
^ Still in test

Impact and Benefits

Advances in oxy-combustion technology will be instrumental in improving power generation efficiency while lowering the amount of CO_2 produced and concentrating the CO_2 effluent streams, making them suitable for carbon capture and sequestration. The Advanced Combustion Project represents an integrated, cross-functional approach and will lead to a better understanding of environmental and mechanical behavior of alloys.

Development of computational materials modeling techniques will aid in alloy design and manufacture, as well as simulating component performance in extreme environments. Subsequent modeling and characterization activities will produce physics-based life prediction models, resulting in optimum utilization of these materials as components. Consequently, integrated characterization modeling will provide tools that can be used to predict environmental degradation and long-term mechanical behavior in oxy-fuel combustion boilers and A-USC steam turbines.

NETL

ADVANCED COMBUSTION **NETL Team Technical Coordinator:** Jeffrey Hawk

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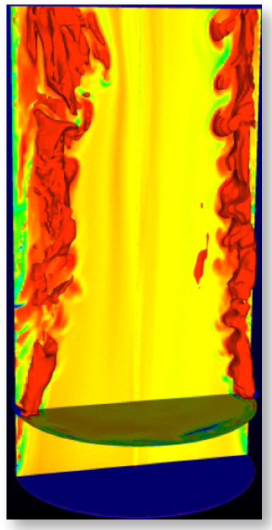
the ENERGY lab

R&D FACTS

Advanced Energy Systems

Advanced Gasification

Carbon feedstock gasification is a promising pathway for high-efficiency, low-pollutant power generation and chemical production. The inability, however, to meet a number of operational goals could create roadblocks to widespread acceptance and commercialization of advanced gasification technologies. We must, for example, achieve gasifier online availability of 85–95 percent in utility applications, and 95 percent for chemical production and other applications so the service life of gasifiers can meet the performance needs of industry. To do so, we need new technologies that address carbon conversion, slag viscosity, and downstream fouling. Technologies that reduce the cost of CO_2 separation and capture are also required.



High Resolution Simulations using NETL's computational models.

The National Energy Technology Laboratory (NETL) Gasification Team and members of the NETL-Regional University Alliance (NETL-RUA) are taking an integrated approach to developing physics-based methods, models, and tools that can support the development and deployment of advanced gasification devices and systems.

AVESTAR™ Center

The NETL Advanced Virtual Energy Simulation Training and Research (AVESTAR™) Center is pursuing a collaborative, innovative, internationally-recognized R&D program to achieve operational excellence in current and next-generation gasification-based power plants, with or without carbon capture. Research has concentrated on developing high-fidelity

AVESTAR™ users making high-fidelity real-time dynamic simulations of an IGCC plant with CO_2 capture.

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URS Corporation

Virginia Tech

West Virginia University

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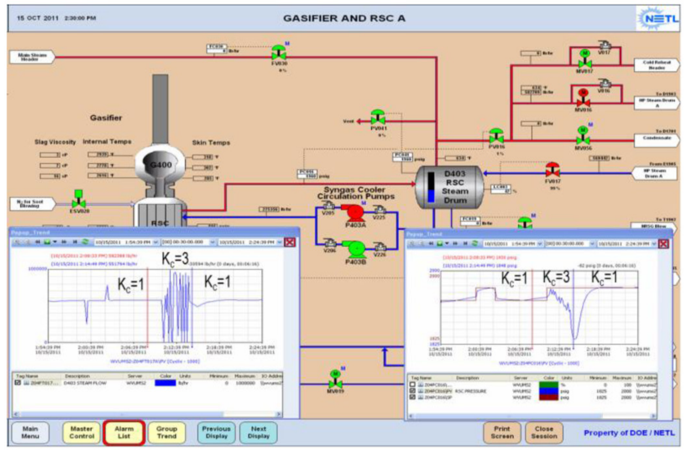
dynamic models of coal-fired gasifiers, the centerpiece of integrated gasification combined cycle (IGCC) power plants. The models maximize the efficiency and profitability from plant operations through process control and by maximizing business value from all plant assets - all while reducing negative environmental impact and improving safety. The AVESTAR™ Center brings together dynamic simulation-based technologies, state-of-the-art facilities, and leading energy researchers. Current R&D efforts are focused on the areas of dynamic process modeling, advanced process control, and optimal sensor placement. AVESTAR™ will also be instrumental in preparing an industry workforce trained to safely and effectively operate, control, and manage commercial-scale IGCC systems with CO_2 capture.

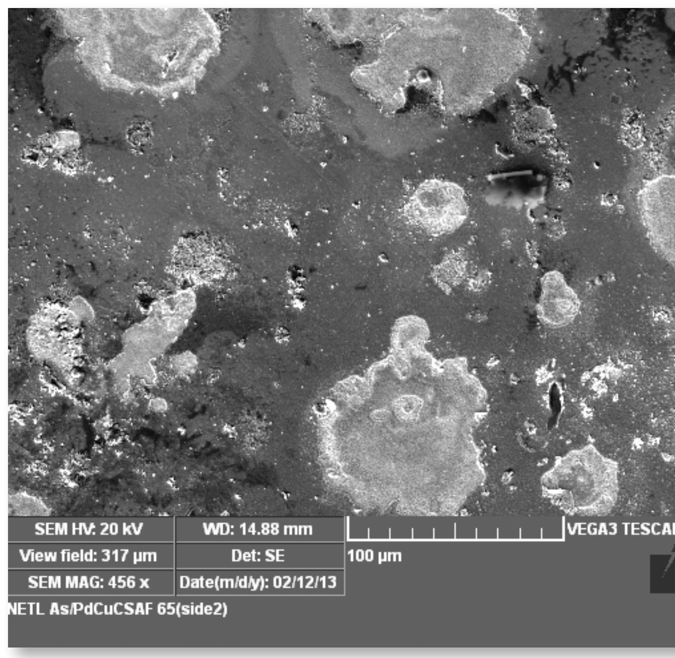
www.netl.doe.gov/avestar



Simulations used to model outcomes in an IGCC plant when making changes in plant operation conditions.

Warm Gas Cleanup

Palladium-based sorbents are among the most promising candidates for the high-temperature, one-step capture of trace elements from coal-derived fuel gases which will reduce the footprint, cost, and complexity of pollution mitigation. NETL research on gas cleanup is focusing on testing and developing palladium sorbents for the capture and removal of trace metals like mercury, arsenic, selenium, phosphorus, and cadmium (co-capture). NETL is also studying the removal and detection of these and other contaminants from fluid streams using techniques that include sorbent, catalyst, analytical, photochemical, and electrochemical methods. Capacity for capture is being determined in simulated fuel gases through the use of laboratory-scale packed-bed reactors and at larger scales in slipstreams of real fuel gas at an actual gasification facility. Warm gas cleanup research promotes the utilization of abundant domestic coal in a clean and environmentally friendly manner. Technology developed under this project will allow gasification to meet stringent EPA regulations for trace metal emissions. Three capture technologies developed by NETL were recently licensed to industry.



Interactions on a precious metal surface coating (white areas) caused by impurities during removal from syngas.

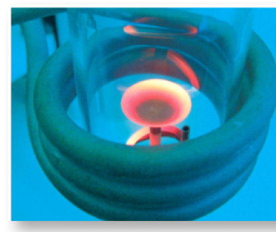
Refractory Improvement

Coal and petcoke, common carbon feedstock in slagging gasifiers, are typically high in mineral impurities, materials which significantly impact slag viscosity and refractory wear. Research aimed at refractory improvement is focused on refractory development and the impact of additives on carbon feedstock ash behavior and refractory wear. Refractory service life improvement through material development or modeling and the control of slag chemistry is being evaluated via laboratory testing at NETL and through the cooperation of industry gasifier operators. Slag management for optimum gasifier service is being accomplished by developing a slag model to allow gasifier operators control of slag viscosity, maximize refractory service life, and minimize downstream material issues like syngas fouling. A modeling program is undergoing evaluation at a commercial gasifier site to control slag properties and minimize refractory wear.

Changes in refractory wear between old technology (left), NETL developed (center), and unused refractory (right) after similar exposure in a commercial gasifier. Less wear in the newly developed refractory will result in longer service life and reduced downtime for gasifier repair.

Low-Rank Coal Optimization

Research in this area focuses on the development of gasification performance prediction models to reduce uncertainties associated with the use of low-rank coals and co-feeds, including low-rank coal and biomass. The development of a hierarchy of co-feed trigonometric models with uncertainty quantification will provide a practical framework for quantifying various types of uncertainties and rank assessing the impact of their gasification through computer models of the physical system. Reducing the uncertainty associated with different carbon feedstock materials will enable designers and operators of gasifiers to predict and understand material behavior prior to utilization, leading to more efficient use of these materials.



Temperature inside the high speed HS-TGA

Conversion and Fouling

Accurate physical models are currently unavailable for predicting and controlling rates of slag buildup in a gasifier and ash deposition in a convective syngas cooler. Problems associated with ash buildup can lead to gasifier shutdown. Plants have experienced problems such as lower carbon conversion and plugging of syngas coolers with fly ash, a problem that can be severe enough to lead to plant shutdown. Overall impact is reduced plant heat recovery, strain on solids handling and grey water circuits, and a reduction in the overall reliability of the gasifier.

Research in this area has focused on establishing how slag iron and vanadium oxide content, as well as oxidation state, impact slag viscosity and is aimed at negating plugging and fouling throughout the syngas cooling system. Control of slag properties will lead to an increased capability to control gasifier performance and to determine the impacts and limits of using various coal grades and petcoke in entrained gasifiers. In addition, development of computational simulation tools will reduce uncertainty associated with the use of low-rank coal and mixed feeds. Results of this work will aid in gasifier design and performance relative to the use of these fuels, allowing for fuel flexibility in current and future gasification facilities.

Convective syngas cooler fouling source
– Global Energy, Inc –

ADVANCED GASIFICATION **NETL Team Technical Coordinator:** James Bennett

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Pisupati, Sarma	PI	PSU	Devolatilization and Char Kinetics Support
Song, Xueyan	PI	WVU	Different Gasifier Liner Wear Support
Song, Xueyan	PI	WVU	High Vanadium Oxide Study Support
Musser, Jordan	PI	WVU	Implement Heat & Mass Transfer to MFIX-PIC Support
Dietiker, Jean-Francois	PI	WVU	MFIX Development Verification and Validation Support
Kuhlman, John	PI	WVU	Model Development Support
Weiland, Nathan Bedick, Clinton	PI Researcher	WVU WVU	Particle Deposition Support
Kuhlman, John Krishnaswamy, Ramalakshmi Varre, Sai Bharath Kumar	PI Grad Student Grad Student	WVU WVU WVU	Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Roy, Christopher Choudhary, Aniruddha	PI Grad Student	VT VT	Uncertainty Quantification and Sensitivity Analysis Support
Gellman, Andrew Miller, James	PI CO-PI	CMU CMU	Warm Gas Cleanup Support

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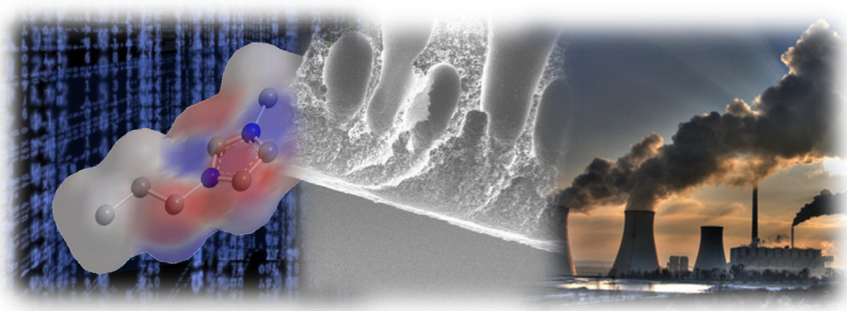
R&D FACTS

Carbon Capture

Carbon Capture Research and Development

Carbon capture and storage from fossil-based power generation is a critical component of realistic strategies for arresting the rise in atmospheric CO_2 concentrations, but capturing substantial amounts of CO_2 using current technology would result in a prohibitive rise in the cost of producing energy. The National Energy Technologies Laboratory-Regional University Alliance (NETL-RUA) is pursuing a multifaceted approach, which leverages cutting-edge research facilities, world-class scientists and engineers, and strategic collaborations to foster the discovery, development, and demonstration of efficient and economical approaches to carbon capture.



Integrated technology development takes materials from molecular design through fabrication to commercialization

Project Overview

The NETL-RUA capture program seeks to create technological solutions for carbon capture from pulverized coal power plants, integrated gasification combined cycle (IGCC) plants, and oxy-fuel combustion plants. Capture conditions are vastly different in each of these power cycles, so separate materials development programs have been undertaken for each. Additionally, both the IGCC and oxy-fuel cycles require large amounts of oxygen, which is expensive to produce and adds considerable cost to the processes. NETL-RUA is also exploring new materials for the selective separation of oxygen from air.

Three approaches have generally been considered for the separation of CO_2 in power generation applications. Solvents and sorbents are materials which selectively sorb CO_2 from gas mixtures and release it after a change in either temperature or pressure, producing a pure stream of CO_2. Membranes are devices which allow CO_2 to pass through and retain all the other components of gas mixtures. Each technology has its own advantages and disadvantages.

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Virginia Tech

West Virginia University

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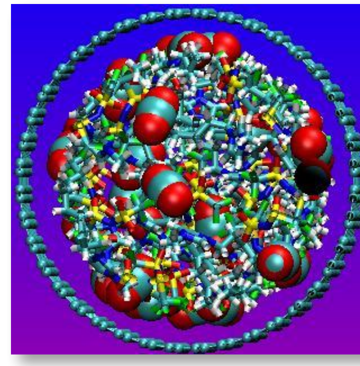
Energy Frontiers Research Center

Lawrence Berkeley National Laboratory

Research Institute of Innovative Energy

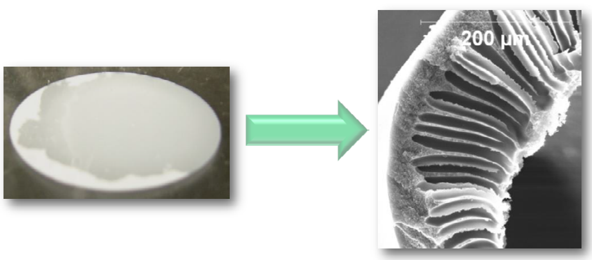
Generally, solvents are the best understood technologies, and the existing commercial products for CO_2 capture are all solvent-based (Selexol, Rectisol, MEA). Sorbents and, particularly, membranes are less developed as CO_2 capture technologies but have the potential for much greater improvements in performance compared to existing technologies. NETL-RUA is examining all three classes of technologies to better address both near and longer term capture goals.



Computational models examine the molecular level interactions of materials and aid in optimization

To accelerate development of solvents, sorbents, and membranes, NETL-RUA is pursuing the complimentary utilization of computational and experimental approaches. For example, atomistic modeling approaches are coupled with surface science experiments to understand and optimize the structure and energetics of materials for the specific application. The resulting molecular-level information can be used as a basis to predict the bulk thermodynamic and kinetic material properties by force-field modeling, Monte Carlo simulation, and molecular dynamics. Validated models are used to predict the performance of materials in the application of interest, thus allowing experimental resources to focus on only the most promising materials. Substances designed using fundamental approaches are synthesized and characterized in NETL-RUA's fully equipped synthetic facilities, and the materials are fabricated into configurations, including thin-film membranes and sorbent particles, to assess their performance at conditions consistent with those encountered in carbon dioxide capture applications.

Researchers work closely with process analysts to provide high quality information required for techno-economic assessments to minimize the erroneous assumptions that are often required when extrapolating laboratory results to plant-scale models. Laboratory results are scaled to the device level, such as a membrane module or sorbent bed, using a combined experimental and computational approach. In this approach, computational fluid dynamics and small-scale device fabrication and testing work hand-in-hand to provide insights into the functional performance that can be expected at the plant scale, including performance degradation and heat- and mass-transfer limitations. The integrated approach, which can be envisioned as a cyclic process ranging from fundamental science through process evaluation, results in an accurate assessment of emerging technologies being developed. Furthermore, this process provides researchers insight into the properties that must be improved in future generations of materials and the scientific limitations bounding technologies. The close relationship of the scientists, engineers, and systems analysts allows each step in the technology development approach to continuously inform the others and produce greater efficiency. This approach continues to provide rapid advancement in the development of several materials including amine-enriched sorbents, ionic liquids, and metal-organic frameworks.



Advanced fabrication and synthetic techniques move conceptual materials toward practical application

Expected Outcomes

The most promising materials, those which appear likely to achieve substantial reductions in the cost of carbon capture, will be further tested at the National Carbon Capture Center or other power generation facilities using actual flue or fuel gas. Technologies, which test favorably under these conditions, will be transferred to industry through joint development and patent licensing. The research described will result in the creation of new materials, characterization of the performance of the materials under realistic conditions, and accelerated commercialization of technologies based on the materials.

Benefits

The research will accelerate the development (ranging from the discovery of innovative materials through evaluation in real systems) of efficient, cost-effective fossil fuel conversion systems that meet the post-combustion programmatic goal of capture of 90% of the CO_2 produced from an existing coal-fired power plant with less than a 35% increase in the cost of electricity (COE) and the pre-combustion goal of 90% CO_2 capture with a less than 10% increase in COE. Materials and separation technologies developed in this research may also have impact in other areas. Reductions in the cost of producing oxygen in particular would be of great value in applications as diverse as chemical production and medicine.

CARBON CAPTURE RESEARCH AND DEVELOPMENT **NETL Team Technical Coordinator:** David Luebke

Name	Project Role	Affiliation
Duan, Yuhua	Physical Scientist	NETL
Fauth, Daniel J	Research Chemist	NETL
Granite, Evan J	Chemical Engineer	NETL
Gray, McMahan L	Physical Scientist	NETL
Hoffman, James S	Mechanical Engineer	NETL
Hopkinson, David	Mechanical Engineer	NETL
Luebke, David R	General Engineer	NETL
Matranga, Christopher	Research Chemist	NETL
Matuszewski, Michael	General Engineer	NETL
Morreale, Bryan	General Engineer	NETL
Myers, Christina R	Chemical Engineer	NETL
Richards, George	Energy Sys Dynamics	NETL
Shadle, Lawrence J	Physical Scientist	NETL
Siefert, Nicholas	Mechanical Engineer	NETL
Siriwardane, Ranjani	Physical Scientist	NETL
Steckel, Janice A	Physical Scientist	NETL
Zandhuis, Paul	Project Lead	URS
Albenze, Erik	Research Engineer	URS
Culp, Jeffrey	Research Scientist	URS
Egbebi, Adefemi	Research Scientist	URS
Hammache, Sonia	Research Engineer	URS
Miller, Russell	Specialist	URS
O'Connor Jr, John	Engineer	URS
Resnik, Kevin	Research Engineer	URS
Shi, Fan	Research Scientist	URS
Thompson, Robert	Research Scientist	URS
Wickramanayake, Wasala	Research Engineer	URS
Shi, Wei	Research Scientist	URS
Lekse, Jonathan	Research Scientist	URS
Hong, Lei	Research Scientist	URS

Name	Project Role	Affiliation	University Project Title
Achary, Damodaran K Allen, Jesse James Mao, Xiaojian	PI Post Doc Post Doc	Pitt Pitt Pitt	Advanced NMR Characterization of Ionic Liquids
Kitchin, John Lee, Anita S	PI Grad Student	CMU CMU	Characterization of the High Pressure Absorption of CO2 into Ionic Liquids
Nulwala, Hunaid	PI	CMU	Chemical Informatics Collaboration
Achary, Damodaran K Allen, Jesse James Mao, James	PI CO-PI CO-PI	Pitt Pitt Pitt	CO2 Sorption Characterization NMR
Janik, Michael J Gao, Hongwei Brady, Brian	PI Researcher Under Grad	PSU PSU PSU	Computational Modeling of Novel Materials for Pre-Combustion CO2 Removal
Enick, Robert M Koronaios, Peter Jordan, Kenneth D Li, Tao	PI Post Doc PI Grad Student	Pitt Pitt Pitt Pitt	Development of High Molecular Weight PDMS
Jordan, Kenneth D Marjolin, Aude Su, Xiaoge Jordan, Kenneth D Marjolin, Aude	PI Post Doc Grad Student PI Post Doc	Pitt Pitt Pitt Pitt Pitt	Development of Polarizable Force Fields for Ionic Liquids
Nulwala, Hunaid	PI	CMU	High Temperature Supported Ionic Liquid Membrane Synthesis - (CMS (CRADA) Funded Carbon Capture Support)
Li, Bingyun Noore, Jabeen	PI Technician	WVU WVU	Hybrid Ionic Liquid Sorbents for Post-Combustion CO2 Capture
Rubin, Edward S	PI	CMU	Integrated Environmental Control Model (IECM)
Kitchin, John	PI	CMU	Investigation and Mechanisitic Study of Amine-Enriched Sorbents
Kowalewski, Tomasz Nulwala, Hunaid Lamson, Melissa	CO-PI CO-PI Grad Student	CMU CMU CMU	Low-viscosity Eutectic Solvents
Rosi, Nathaniel L	PI	Pitt	Metal Organic Synthesis
Venna, Surendar Reddy	PI	WVU	Mixed Matrix Membrane Casting Technique Development
Johnson, J Karl Zhang, Bo Rothrauff, Bartholomew	PI Grad Student Under Grad	Pitt Pitt Pitt	Molecular Modeling of Ionic Liquids for Post-Combustion CO2 Capture Solvents
Natesakhawat, Sittichai	PI	Pitt	Nitrogen Rich Porous Nanocarbon Materials
Kowalewski, Tomasz Mohin, Jake Lamson, Melissa	PI Grad Student Grad Student	CMU CMU CMU	Nitrogen Rich Porous Nanocarbon Materials

Continued on next page

CARBON CAPTURE RESEARCH AND DEVELOPMENT **NETL Team Technical Coordinator:** David Luebke

Name	Project Role	Affiliation	University Project Title
Enick, Robert M	PI	Pitt	PDMS Characterization and Testing
Koronaios, Peter	Post Doc	Pitt	
Nulwala, Hunaid	PI	CMU	PDMS Formulation
Li, Bingyun	PI	WVU	Phase Change Amino Acid Development
Wang, Xianfeng	Post Doc	WVU	
Kitchin, John	PI	CMU	Raman Studies Examining Contamination Effects
Hallenbeck, Alex	Grad Student	CMU	
Lee, Anita S	Grad Student	CMU	
Johnson, J Karl	PI	Pitt	Reactive Force Field Development
Bajura, Richard A	PI	WVU	Research Support for Pre-Combustion Membrane Ring-complexing Supported Ionic Liquid Membranes
Venna, Surendar Reddy	CO-PI	WVU	
Venna, Surendar Reddy	PI	WVU	Single Crystal Permeation Measurement Technique
Matyjaszewski, Krzysztof	PI	CMU	Structure Formation via Block Co-Polymerization
He, Hongkun	Grad Student	CMU	
Rosi, Nathaniel L	PI	Pitt	Structure Formation via Nanopore Confinement
Matyjaszewski, Krzysztof	PI	CMU	Synthesis and Characterization of Di-Block Polymers with Nano-Scale Ordered Structures
He, Hongkun	Grad Student	CMU	
Nulwala, Hunaid	PI	CMU	Synthesis of Ring-Complexing Ionic Liquids

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R&D FACTS

Computational Energy Science

Carbon Capture Simulation Initiative

The Carbon Capture Simulation Initiative (CCSI) is a partnership among national laboratories, industry, and academic institutions including members of the NETL-Regional University Alliance (NETL-RUA) to develop and deploy state-of-the-art computational modeling and simulation tools to accelerate the development of carbon capture technologies from discovery to development, demonstration, and ultimately the widespread deployment to hundreds of power plants. The CCSI Toolset will provide industry end users with a comprehensive, integrated suite of scientifically validated models, with uncertainty quantification, optimization, risk analysis, and decision-making capabilities. The CCSI Toolset will incorporate commercial and open-source software currently in use by industry and develop new software tools as necessary to fill technology gaps identified during project execution.

The CCSI Toolset will—

- Enable quicker identification of promising concepts through rapid computational screening of devices and processes.
- Reduce the time to design and troubleshoot new devices and processes.
- Quantify the technical risk in taking technology from laboratory to commercial scale.
- Stabilize deployment costs more quickly by replacing some of the physical operational tests with virtual power plant simulations.

Project Overview

The ultimate goal of CCSI is to deliver the CCSI Toolset, which will provide new models and computational capabilities that will accelerate the commercial development of carbon capture technologies and a broad range of technology development in general (power, refining, chemicals production, gas production, etc.). The CCSI Toolset will ultimately consist of new computational tools and models including:

- Basic Data submodels, which include the ability to quantify the uncertainty in the models and parameters representing chemical kinetics, diffusion and equilibrium.
- High resolution filtered submodels to capture the effects of phenomena, which are too small to resolve directly in large scale simulations.
- Validated high-fidelity CFD models, which enable a detailed understanding of the internal behavior of materials inside of complex equipment, coupled with a framework to quantify the effects of uncertainty on simulation results.
- Steady state and dynamic process models which can be used for screening new concepts and understanding how equipment behaves as an interacting system.
- Process synthesis, design, optimization and uncertainty quantification (UQ) tools for developing optimal processes and quantifying the effects of uncertainty in models and model parameters.

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Lawrence Berkeley National Laboratory

Lawrence Livermore National Laboratory

Los Alamos National Laboratory

Pacific Northwest National Laboratory

Princeton University

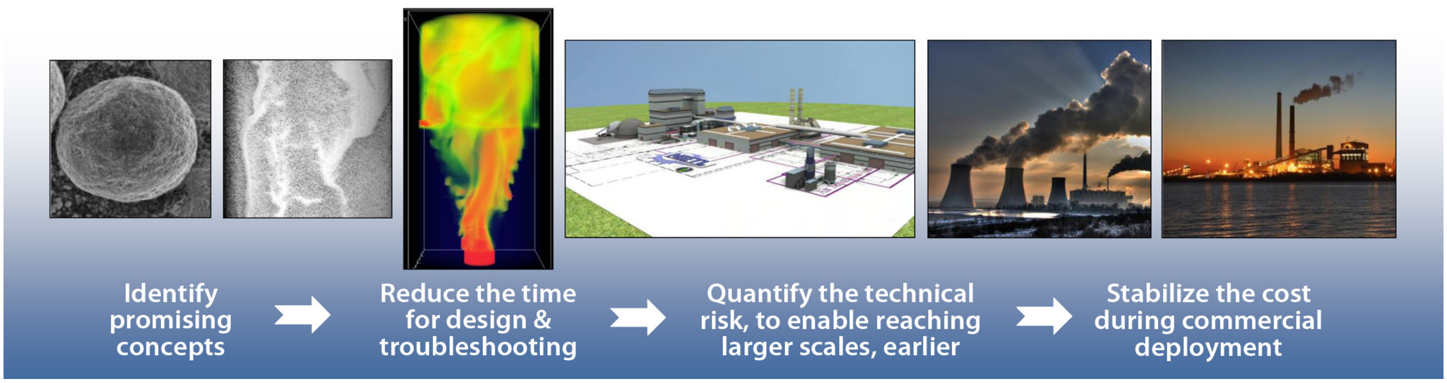
U.S. DEPARTMENT OF ENERGY

- An integrated framework for dynamics and control which will enable users to develop optimal control strategies.
- A risk analysis and decision making framework, which brings together concepts of Technology Readiness Levels (TRL), technical and financial risk into an interface, which couples each risk component, enables the transfer of information between the components, and displays the risk analysis results.
- Data management and other integration tools.

An initial release of the CCSI Toolset in September 2012 consisted of:

- New tools for process synthesis and optimization to help identify promising concepts more quickly.
- New physics-based models of potential capture equipment and processes that will reduce the time to design and troubleshoot new systems.
- A framework to quantify the uncertainty of model predictions.
- Various enabling tools that provide new capabilities such as:
  - creating reduced order models (ROMs) from reacting multiphase flow simulations, and
  - running thousands of concurrent process simulations concurrently for optimization and uncertainty quantification.

To provide a framework around which the toolset can be developed and demonstrated, CCSI initially focused on an industrially relevant challenge problem (ICP) related to post-combustion capture by solid sorbents. A second ICP related to post-combustion capture by advanced solvent systems will also be incorporated beginning in 2013.



Impacts and Benefits

Over five years, CCSI will provide Technology Developers and Plant Operators with a validated suite of models and simulation tools that enable the rapid development and deployment of new carbon capture technologies. The CCSI toolset will provide tools and methodologies that accurately predict the performance of equipment and processes; reduce the uncertainty associated with system integration and scale-up; and accelerate the commercial development of integrated carbon capture technologies. The CCSI toolset will include validated models of carbon capture equipment and processes as well as new design and analysis tools and methodologies. Industry utilizing the CCSI toolset will be able to reduce the time and expense of new technology development, from discovery to demonstration to widespread deployment, by a minimum of five years. The total cost savings that could be realized by using the CCSI toolset to scale up and widely deploy just one carbon capture technology is estimated to be approximately $500 million (net present value basis).

Another objective of CCSI is to use information from science-based models with quantified uncertainty to inform investors. Validating the models at different scales, quantifying the uncertainty of model predictions, and estimating the technical risk will enable smarter demonstrations and ultimately could accelerate demonstrations by several years.

CCSI fits within the larger National Energy Technology Laboratory (NETL) CCUS research, development, and deployment (RD&D) program. The CCUS RD&D program will be a rich source of data for validating models in the CCSI Toolset. For the post-FY15 phase, the CCSI Toolset will add value to the overall carbon capture effort through the acceleration of analysis of process design and integration options as 2nd generation technology is scaled from pilot to demonstration scale.

CCSI Carbon Capture Simulation Initiative | Berkeley Lab | Lawrence Livermore National Laboratory | Los Alamos National Laboratory EST. 1943 | Pacific Northwest National Laboratory | NETL

CARBON CAPTURE SIMULATION INITIATIVE (CCSI) **NETL Team Technical Coordinator:** David Miller

Name	Title	Affiliation
Miller, David C	General Engineer	NETL
Zitney, Stephen E	General Engineer	NETL
Syamlal, Madhava	Focus Area Leader	NETL
Carney, Janine	General Engineer	NETL
Cottrell, Roger	Project Lead	URS
Moore, Kevin	Project Lead	URS
Ma, Jingliang	Research Engineer	URS
Mahapatra, Priyadarshi	Research Engineer	URS

Name	Project Role	Affiliation	University Project Title
Dietiker, Jean-Francois	PI	WVU	CCSI Element 2 - Particle & Device Scale Models (NETL) MFIX Development
Mebane, David	PI	WVU	CCSI Team – Element 1 Basic Data and Models
Grossmann, Ignacio	PI	CMU	NETL CCSI Team – Element 3: Process Synthesis & Design
Chen, Yang	Post Doc	CMU	
Eslick, John	Post Doc	CMU	
Biegler, Lorenz	PI	CMU	Professional Services for Advanced Research (AR) Carbon Capture Simulation Initiative (CCSI) in support of Element 3 –Process Synthesis and Design
Dowling, Alexander	Grad Student	CMU	
Grossmann, Ignacio	PI	CMU	
Yang, Linlin	Grad Student	CMU	
Sahinidis, Nikolaos V	PI	CMU	
Yuan, Zhihong	Post Doc	CMU	
Cozad, Alison	Grad Student	CMU	
Siirola, Jeffrey	PI	CMU	
Bhattacharyya, Debangsu	PI	WVU	Professional Services for Advanced Research (AR) Carbon Capture Simulation Initiative (CCSI) in Support of Element 4-Plant Operations and Control
Modekurti, Srinivasarao	Post Doc	WVU	
Rubin, Edward S	PI	CMU	Professional Services for Advanced Research (AR) Carbon Capture Simulation Initiative (CCSI) in support of the Executive Committee
Bhattacharyya, Debangsu	PI	WVU	Sensor placement algorithm for at least one section in an IGCC plant with CO2 capture
Turton, Richard	CO-PI	WVU	
Paul, Prokash	Grad Student	WVU	

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R & D FACTS

Carbon Storage

Carbon Storage Research

Carbon capture and storage (CCS) is a key component of the U.S. carbon management portfolio. Numerous studies have shown that CCS can account for up to 55 percent of the emissions reductions needed to stabilize and ultimately reduce atmospheric concentrations of CO_2.

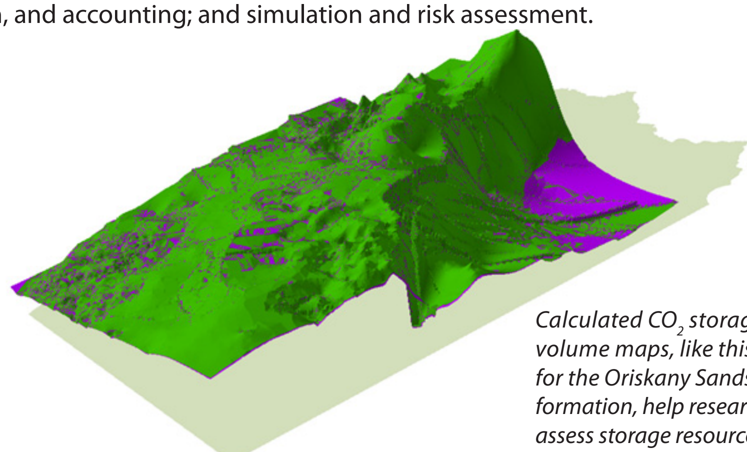
NETL's Carbon Storage Program is readying CCS technologies for widespread commercial deployment by 2020. The program's goals are:

- By 2015, develop technologies that can separate, capture, transport, and store CO_2 with a less than 10 percent increase in energy costs.
- By 2015, develop technologies to help industry predict CO_2 storage capacity in geologic formations with a ± 30 percent margin of error.
- By 2015, develop technologies to verify that 99 percent of injected CO_2 remains in injection zones.
- By 2020, complete a series of best practices manuals for site selection, characterization, and operations and closure practices.

Core R&D Under NETL's Carbon Storage Program

NETL's is conducting a range of projects under the Carbon Storage Program's Core R&D element, one of three program elements that also include Infrastructure and Global Collaborations. Members of the NETL-Regional University Alliance (NETL-RUA) collaborate with NETL's Office of Research and Development (ORD) on these projects.

ORD's activities involve applied laboratory and pilot-scale experiments as well as numerical modeling. Projects encompass three of five Core R&D technical focus areas for CCS technology and protocol development: geologic storage; monitoring, verification, and accounting; and simulation and risk assessment.



Calculated CO_2 storage volume maps, like this one for the Oriskany Sandstone formation, help researchers assess storage resources.

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URS Corporation

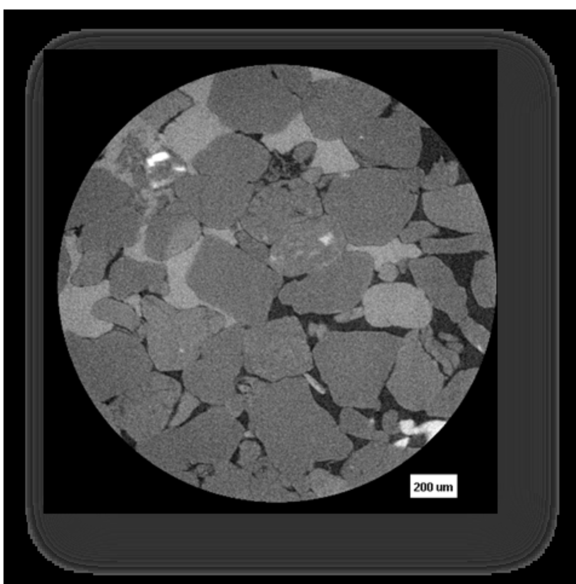
Virginia Tech

West Virginia University

Proposed Research

Research tasks are organized into five theme areas to address key research needs as outlined in NETL's *Carbon Sequestration Program: Technology Program Plan*.

- **Flow properties of reservoirs and seals**—Assessing the impact of chemical reactions and geomechanics on injectivity and storage permanence.
- **Fundamental processes and properties**—Improving our ability to predict capacity, injectivity, and storage permanence by better understanding reaction kinetics and fluid properties.
- **Estimates of storage potential**—Evaluating, improving, and expanding current methodologies for predicting storage capacity to improve accuracy and allow for use in alternative reservoirs.
- **Verifying storage performance**—Improving subsurface and near-surface monitoring technologies through verify storage permanence and track plume movement.
- **Geospatial data resources**—Developing resources to improve access to geospatial data for public use (NATCARB), as well as for researchers.



A micro-CT image of a sample reservoir rock structure.

ORD Objectives and Expected Benefits Under Core R&D

Research being conducted by ORD in collaboration with NETL-RUA will enable the development of technologies that will significantly improve the safety and permanence of geologic CO_2 storage.

Objectives include:

- **Geologic storage**—Refine methodology for capacity estimation and determine the geochemical and geo-mechanical impacts on capacity, injectivity, and storage permanence.
- **Monitoring, verification, and accounting**—Develop technologies and techniques to track CO_2, brine, and pressure plume migration in the deep subsurface, into groundwater aquifers, and into the atmosphere.
- **Simulation and risk assessment**—Improve predictions for chemical and biological processes that can impact porosity and permeability of reservoirs and natural seals.

Expected benefits include:

- **Multiphase flow in reservoirs and seals**—Improved models for predicting reservoir performance (injectivity, capacity, and permanence) based on mineralogy, mech-anical stresses, water chemistry, and microbial community. Site-specific assessments of reservoir and seal flow properties.
- **Fundamental processes and properties**—Improved representation of fluid properties and reaction kinetics relevant to storage performance.
- **Estimates of storage potential**—A capacity-estimates model adapted to unconventional storage systems (shales, coal seams, etc.) and CO_2 enhanced oil recovery.
- **Verifying storage permanence**—Methods to ensure storage permanence, including detecting leakage to the surface or groundwater aquifer; tracking CO_2 and pressure plume mitigation in the deep subsurface; and evaluating caprock integrity.
- **Geospatial data resources**—Continuous improvement of the National Carbon Sequestration Database and Geographic Information System (NATCARB), NATCARB website, and future editions of the *Carbon Storage Atlas of the United States and Canada*, as well as the develop-ment of a geospatial database for research use.

R&D163 February 2012

CARBON STORAGE RESEARCH **NETL Team Technical Coordinator:** Brian Strazisar

Name	Title	Affiliation
Bromhal, Grant S	General Engineer	NETL
Cardone, Carol R	Physical Scientist	NETL
Diehl, J Rodney	Physical Scientist	NETL
Dilmore, Robert M	General Engineer	NETL
Edenborn, Harry M	Research Microbiologist	NETL
Goodman Hanson, A	Physical Scientist	NETL
Gulliver, Djuna M	ST (General Eng)	NETL
Hakala, Jacqueline A	Physical Scientist	NETL
Hammack, Richard	Physical Scientist	NETL
Hedges, Sheila W	Research Chemist	NETL
Kutchko, Barbara G	Physical Scientist	NETL
Lopano, Christina	Physical Scientist	NETL
McIntyre, Dustin L	Mechanical Engineer	NETL
McLendon, Thomas	General Engineer	NETL
Mroz, Thomas H	Geologist	NETL
Romanov, Vyacheslav	Physical Scientist	NETL
Rose, Kelly K	Geologist	NETL
Sams III, James I	Hydrologist	NETL
Schroeder, Karl T	Physical Scientist	NETL
Seol, Yongkoo	Physical Scientist	NETL
Soeder, Daniel J	Physical Scientist	NETL
Soong, Yee	Chemical Engineer	NETL
Strazisar, Brian R	Physical Scientist	NETL
Tran, Phuoc X	Mechanical Engineer	NETL
Verba, Circe A	ST(Phys Scientist)	NETL
Wells, Arthur W	Research Chemist	NETL
Myshakin, Eugene	Project Lead	URS
King, Seth	Project Lead	URS
Haljasmaa, Igor	Project Lead	URS
Crandall, Dustin	Project Lead	URS
Lindner, Ernest	Project Lead	URS
Disenhof, Corrine	Project Lead	URS
Magdelena Gill	Scientist	URS

Name	Project Role	Affiliation	University Project Title
Karamalidis, Athanasios	PI	CMU	Arsenopyrite Precipitation and Dissolution Studies
Small, Mitchell J Thomas, Andrew Popova, Olga H	PI CO-PI Grad Student	CMU CMU CMU	Compare methodologies by applying to site such as Illinois basin or Oriskan
Gao, Dengliang Babarsky, Albert Di, Haibin	PI Grad Student Grad Student	WVU WVU WVU	Developing and applying new seismic waveform attributes to detect fractures
Vesper, Dorothy J Riddell, Jill	PI Grad Student	WVU WVU	Development of field CO2 Measurement Methods
Westman, Erik Sun, Enji	PI Post Doc	VT VT	Double difference tomography to detect plume locations using seismic activity
Harbert, William	PI	Pitt	Effects of pore-filling fluids on seismic wave properties
Small, Mitchell J Thomas, Andrew Popova, Olga H	PI CO-PI Grad Student	CMU CMU CMU	Evaluate implications of storage estimates based on more detailed spatial parameters using DOE assessment mehodology
Karpyn, Zuleima T Cao, Peilin	PI Grad Student	PSU PSU	Experimental Investigation of Conditions Affecting Wellbore Integrity due to Chemical Reaction Using X-ray microCT Imaging
Harbert, William	PI	Pitt	Field data analysis determining the location of CO2 in the reservoir
Karamalidis, Athanasios	PI	CMU	Geochemical Effects Inter-lab Round Robin
Gregory, Kelvin B Lowry, Gregory Victor	CO-PI CO-PI	CMU CMU	Impact of Microbial Mediated Precipitation on Flow and Seal Properties
Burbey, Thomas J	PI	VT	Interpreting mechanical responses from a reservoir to determine pressure change
Karamalidis, Athanasios	PI	CMU	Laser Induced Breakdown Spectroscopy (LIBS) online experiments and analysis
Carr, Timothy Robert Sharma, Maneesh Chen, Xiannian Kramer, Christian T Donaldson, Kurt A Fedorko, Evan J LaFone, Frank Shaffer, Cory	PI CO-PI Researcher Graduate Technician Technician Technician Technician	WVU WVU WVU WVU WVU WVU WVU WVU	NATCARB Database and Viewer Development

Continued on next page

CARBON STORAGE RESEARCH **NETL Team Technical Coordinator:** Brian Strazisar

Name	Project Role	Affiliation	University Project Title
Stewart, Brian W	PI	Pitt	Natural isotope tracers for quantitative MVA
Capo, Rosemary C	PI	Pitt	
Nakles, David V	PI	CMU	Risk assessment in CO2 geologic sequestration
Small, Mitchell J	CO-PI	CMU	
Azzolina, Nicholas	Grad Student	CMU	
Brantley, Susan L	PI	PSU	Sensitivity of mineral solution rates in reactive transport models
Sharma, Shikha	PI	WVU	Tracking CO2 using stable isotope indicators
Mier, Bethany	Grad Student	WVU	
Karamalidis, Athanasios	PI	CMU	Use of Organic Compounds to Track CO2 migration from CO2-EOR (or other storage) Sites

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R&D FACTS

Materials Science

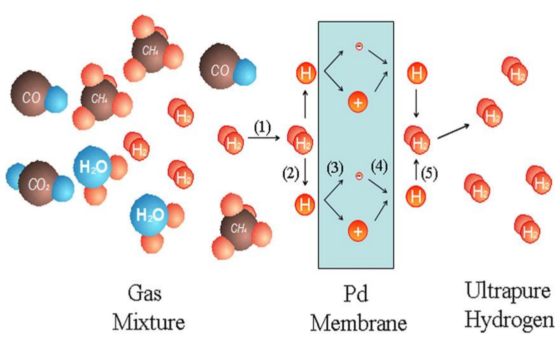
Fuels

Gasification will likely be the cornerstone of future energy and chemical processes due to its flexibility to accommodate numerous feedstocks such as coal, biomass, and natural gas, and to produce a variety of products, including heat and specialty chemicals. Advanced integrated gasification combined cycle schemes require the production of clean hydrogen to fuel innovative combustion turbines and fuel cells.

This research will focus on development and assessment of membranes tailored for application in severe environments associated with syngas conversion. The overall objective is to make significant advances toward developing low-cost membrane materials and architectures that have high hydrogen selectivity, provide high hydrogen fluxes, and resist degradation by syngas-laden contaminants. The NETL-Regional University Alliance (NETL-RUA) Hydrogen and Clean Fuels Project will focus on development of hydrogen separation technologies tailored for conditions consistent with post-warm gas cleaning and integration into water-gas shift technologies. Development and demonstration of syngas conversion technologies will facilitate the advancement of affordable fuels, intermediate chemicals, and power from coal-based feeds.

Proposed Fuels Research at NETL

Designing metallic alloys for hydrogen separation membranes applicable to the elevated temperatures in a syngas environment poses significant challenges. In terms of bulk structure, a membrane microstructure that demonstrates long-term stability at high operating temperatures is required. The structure needs to have high solubility and diffusivity for hydrogen atoms, allowing fluxes capable of meeting performance targets in real gas environments. Other significant challenges are related to the surface of the membrane alloys. The alloy surface is required to have catalytic activity for hydrogen dissociation and to maintain this activity for extended periods of time. However, at elevated temperatures, the syngas environment poses opportunities for various reactions to take place on the surface of metals. Syngas species containing oxygen,



Simple schematic of a hydrogen separation palladium (Pd) membrane

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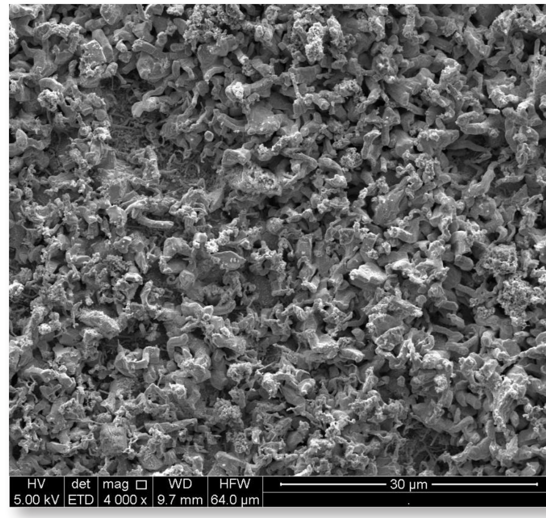
U.S. DEPARTMENT OF ENERGY

sulfur, and carbon have been shown to have deleterious effects on membrane surfaces. Therefore, the alloy surface has to be extremely resistant to these reactions to maintain high catalytic activity. Development of a more durable membrane that can withstand and function under real operating conditions may be more important than focusing on a flux goal. While membranes must still have desirable flux properties, thicker membranes that are more stable at higher temperatures may, relative to cost, be of greater value.

This research will focus on elevated temperature conditions where high efficiencies of separation are possible, and effects of sulfur species are minimized. The proposed three-year project is aimed at providing a design basis for a robust hydrogen separation module based on metal membrane technology. This NETL-RUA Hydrogen and Clean Fuels Project will incorporate an integrated approach, combining computational study, laboratory experimentation, and coupon/slip-stream exposure of membrane alloys for use in syngas environments. Specific research efforts will focus on understanding the following—



Surface of a palladium-based membrane alloy showing the growth of sulfides that occurred during exposure in a gasifier

- The influence of hydrogen sulfide on surface catalytic activity.
- Surface stability within syngas environments.
- Bulk stability and bulk transport, which includes any effect of surface products.
- The knowledge-base’s application to design and optimization of a membrane module.
- Opportunities for the integration of membrane technologies into other unit operations.
- Novel membrane materials identified for use in syngas environments.

The successful execution of this research will result in an advanced understanding of bulk and surface chemical phenomena that influence membrane performance and the design of engineered materials tailored for operation in syngas environments.

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Ciocco, Mike	Project Lead	URS
Smith, Mark	Project Lead	URS
Abdelsayed, Victor	Research Scientist	URS
Floyd, Donald	Scientist	URS
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Enick, Robert M	PI	Pitt	Task 331 Membrane Reaction Process for Conversion of Coal-Gas Components
Enick, Robert M	PI	Pitt	Task 332 Model Development
Veser, Goetz Natesakhaw at, Sittichai	PI Grad Student	Pitt Pitt	Task 333 Catalytic Processes for Conversion of Coal-Gas
Bajura, Richard A	PI	WVU	Task 4.0 Module Design
Belmaggio, Sharon	Technician	WVU	Task 4.0 Module Design
Franks, How ard L. Jr	Technician	WVU	Task 4.0 Module Design

Fuel Cells

The Solid State Energy Conversion Alliance (SECA) program is responsible for coordinating Federal efforts to facilitate development of a commercially relevant and robust solid oxide fuel cell (SOFC) system. Specific objectives include achieving an efficiency of greater than 60 percent, meeting a stack cost target of $175 per kW, and demonstrating lifetime performance degradation of less than 0.2 percent per 1000 hours over a 40,000 hour lifetime.

The NETL-Regional University Alliance (NETL-RUA) Fuel Cell Project performs fundamental SOFC technology evaluation, enhances existing SOFC technology, and develops advanced SOFC concepts in support of the SECA program. Research projects are designed to meet critical technology development needs that can be uniquely addressed by NETL-RUA and are broadly focused on investigation of the degradation processes of anode/electrolyte/cathode (AEC) components, cathode materials and microstructural engineering, and catalytic fuel reforming. The research approach for each component task is targeted to address SECA program technology development goals, especially with regard to reducing stack costs, increasing cell efficiency, and increasing stack longevity. The ultimate goal of these research and development efforts is to transfer technology that facilitates commercial acceptance of SOFC technology.

Advanced Fuel Cell Research at NETL

Cell and Stack Degradation

Among stack components, the AEC degradation rate is potentially the most influential over the total stack degradation rate. It is also perhaps the most complex in terms of the unique degradative modes, and is also the most susceptible to degradation owing to its central role in the electrochemical process. The AEC is therefore a key component targeted for degradation investigation.

Comprehensive models predicting SOFC stack degradation do not exist, or are not sufficiently descriptive to consider all of the primary degradative modes. Due to the complexity and sheer number of degradation processes occurring in the SOFC stack, the present effort to evaluate degradation is initially confined to the AEC structures and materials under commercial consideration. Results of the degradation mode investigation will be incorporated into a computational model that will include only the most prominent degradation modes. Individual degradation modes will be constituted as mathematical expressions relating dependent AEC parameters (e.g., electrode porosity) to independent operating parameters including operating temperature and local overpotential. This model will provide evolving AEC performance parameter updates on a 40 plus kilohour timescale. Model predictions will be confirmed by comparison to samples prepared in-house and also from samples obtained from industry teams.

A detailed investigation of the degradation modes in the AEC will facilitate targeted efforts to improve fuel cell longevity, ultimately resulting in decreased system costs. Development of a world-class modeling tool will accelerate AEC materials and structure innovation leading to more commercially relevant SOFC technology.

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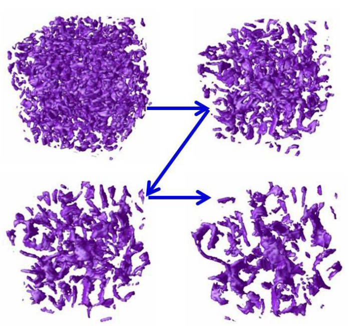
Cathode Materials and Microstructural Engineering

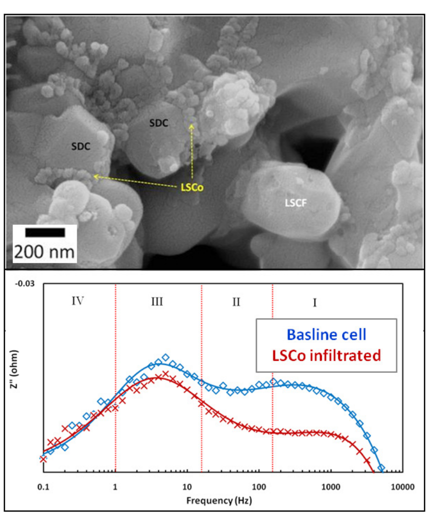
Cathodes are a primary source of the inefficiency observed in a state-of-the-art anode-supported cell operating at temperatures from 750–800 °C. Owing to the relatively high contribution of cathode overpotential to total cell inefficiency, SOFC research to improve cathode performance can help meet critical program targets for cell cost and efficiency.

Conventional cathode microstructural engineering is accomplished through careful control of precursor cathode materials. Using conventional methods, limited variability is available in the final cathode structures. New approaches focus on generation of advanced microstructures that are more conducive to species transport, or methods to apply an engineered cathode at lower cost. These research projects will result in full characterization of performance and durability of the proposed technologies at an intermediate scale. Results will be shared with SECA industrial partners, and the most promising technologies will be selected for further scale-up. Methods developed will generate more functional cathode structures to facilitate enhanced cathode performance, and will potentially allow greater tuning of the final cathode architecture.

These research efforts will improve cathode performance, thereby resulting in increased cell efficiency and, ultimately, a diminished system cost. Cathode material and structure innovations developed through these projects should be readily transferable to industry.



Theoretical degradation and collapse of active regions (triple phase boundaries) in a SOFC cathode simulated for extended operations.

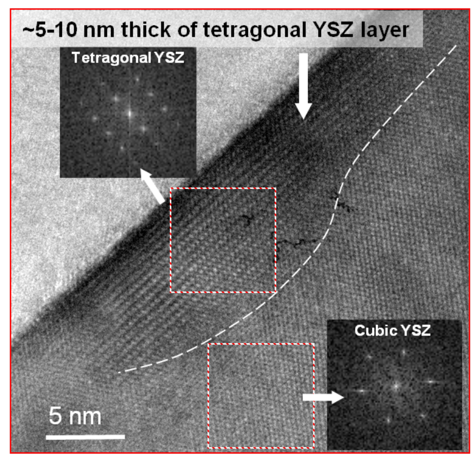


Scanning electron microscopy image of a SOFC cathode infiltrated with electrocatalytic material accompanied by an example of impedance data demonstrating improvement in electrochemical performance (reduced impedance).

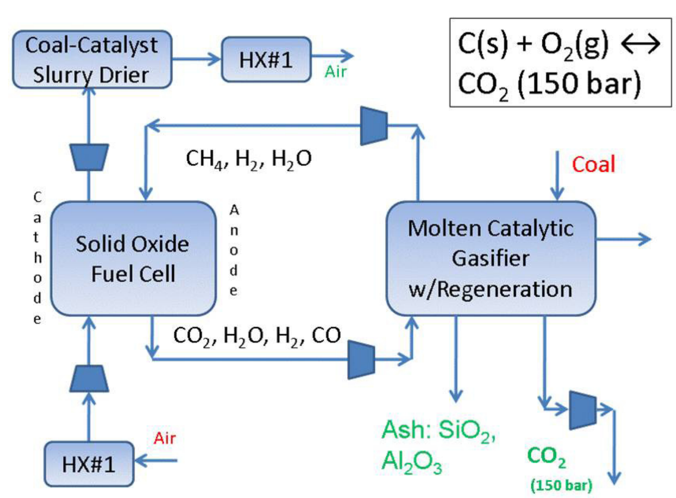
Catalytic Gasification and Fuel Reforming

Recent system studies indicate that coal-to-electricity system efficiencies can approach 60 percent while capturing CO_2, minimizing water consumption, and generating an inflation-adjusted, internal rate of return on investment of over 10 percent per year. One of the keys to achieving this target is production of a high methane synthesis gas of greater than 25 percent from coal gasification. Information collected in the molten catalytic gasification experiments will be used to calculate the gasifier's system efficiency. This project will measure the rates of reaction for the formation of methane in steam-coal gasification in the presence of molten salts as catalysts. Reaction rates and gas compositions will be integrated into gasification numerical simulations to determine the sizing and cost of developing molten catalytic gasifiers for subsequent incorporation into SOFC-based coal power plants.

This catalytic gasification work will facilitate further modeling and analysis of industrial-scale processes aiding the deployment of advanced catalytic gasification technology.



High resolution transmission electron microscopy image of ionic carrier phase breakdown at grain interfaces within a SOFC anode.



Simplified flow diagram of an integrated gasification-SOFC system featuring an advanced molten catalytic gasifier.

FUEL CELLS **NETL Team Technical Coordinator:** Kirk Gerdes

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Chen, Yun	Researcher	WVU	
Mebane, David	PI	WVU	Bayesian Statistical Model of Degradation
Finklea, Harry	PI	WVU	Cathode cation segregation
Chen, Xiaoke	Grad Student	WVU	
Jony, Mahfuzur	Grad Student	WVU	
Chen, Long-Qing	PI	PSU	Cathode evolution by coarsening
Liang, Linyun	Post Doc	PSU	
Song, Xueyan	PI	WVU	Cathode intergranular phase growth analysis
Chen, Yun	Researcher	WVU	
Celik, Ismail B	PI	WVU	Dynamic 3D multi-physics cathode/anode model
Pakalapati, Suryanarayana Raju	CO-PI	WVU	
Song, Xueyan	PI	WVU	Evaluation of electrolyte degradation
Chen, Yun	Researcher	WVU	
Salvador, Paul	PI	CMU	FIB-SEM microstructure reconstructions
Picard, Yoosuf Neelam	CO-PI	CMU	
Bhattacharya, Sudip	Post Doc	CMU	
Liu, Xingbo	PI	WVU	Oxygen reduction reaction model
Zhang, Hui	Researcher	WVU	
Sabolsky, Edward	PI	WVU	Scale-up of engineered foam cathode to SECA scale
Ozmen, Ozcan	Grad Student	WVU	

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R&D FACTS

Crosscutting Research

Industrial Carbon Management Initiative (ICMI)

Background

The ICMI project is part of a larger program called Carbon Capture Simulation and Storage Initiative (C2S2I). The C2S2I has a goal of expanding the DOE's focus on Carbon Capture Utilization and Storage (CCUS) for advanced coal power systems and other applications, including the use of petroleum coke as a feedstock for the industrial sector. The American Recovery and Re-Investment Act (ARRA)-funded work supports the President's stated goal of aggressively reducing our country's energy-related Greenhouse Gas emissions by 83 percent by 2050 from a 2005 baseline. Our nation will immediately see benefits that are directly attributable to projects resulting from the ARRA-funded work.

ICMI is developing carbon management strategies for industrial sources. Industrial sources are typically smaller sources of Carbon Dioxide (CO_2) than base-load power plants and may offer unique options for CO_2 capture, storage, or re-use. While the focus of the research is industrial applications, results are expected to benefit coal power generation, as well.

Research Thrusts

ICMI has three major research thrusts:

- Chemical Looping Technology Development – Chemical looping is a promising approach to generate heat in a combustion process while producing a concentrated CO_2 stream to facilitate carbon capture. Chemical looping research efforts can be categorized as: modeling tool development, experimental work, oxygen carriers research, sensor development, and evaluation of hydrogen production using chemical looping.
- Carbon Storage in Depleted Shale Formations – The potential for CO_2 storage in organic-rich shale formations that have been depleted of natural gas through primary production is being investigated. A secondary focus, enhanced gas production, will be addressed as well. Shale storage efforts can be categorized as empirical characterization of CO_2/shale interactions, simulation of CO_2 storage and enhanced gas recovery potential, and assessing the economic viability of this CO_2 management alternative.
- Photoactive Material (PAM) for Industrial Carbon Management – Catalytic and "photo-catalytic" materials will be studied to assess their potential for using energy from rejected heat or even visible light to convert CO_2 to useful chemicals. In specific industrial settings, this concept might exploit otherwise wasted heat

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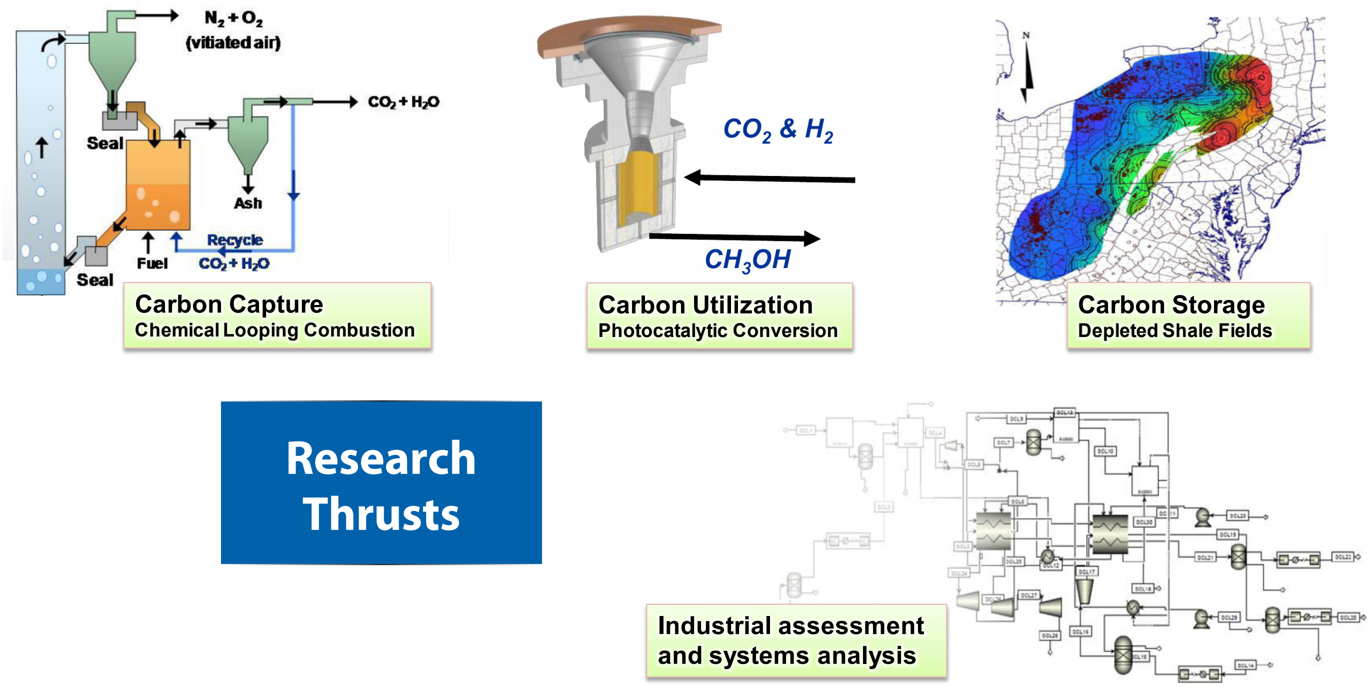
or sunlight to power the chemical reactions. The focus of the work will be characterizing the scientific behavior of new materials so specific industrial applications can be evaluated.

A small, exploratory research component is also included in the ICMI effort because of its potential applicability for integration with industrial processes using saline formations for CO_2:

- Saline Water Treatment Using Clathrate Hydrates – Pumping saline water during CO_2 injection is one means by which the movement of CO_2 can be controlled and pressure relieved from the formation. Research is being conducted on the treatment of highly saline water using clathrate hydrates formed by injection of CO_2 into a reactor at temperatures and pressures conducive to hydrate formation. Findings will contribute to understanding tradeoffs between costs associated with saline formation extracted water management and potential benefits associated with formation pressure management.

Systems Analysis

A critical element of ICMI is the development of CCUS technology that can be used in industrial applications with the eventual goal of application to larger coal-based systems. A combination of industrial market analysis, technology considerations, and techno-economic system models and analysis will be used to identify, assess, and down-select the most promising industrial applications that might use CL, CO_2 storage in spent shale, or re-use.



INDUSTRIAL CARBON MANAGEMENT INITIATIVE (ICMI) **NETL Team Technical Coordinator:** Doug Straub

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Siriwardane, Ranjani	Lead - Element 350	NETL
Summers, Cathy	Lead - Element 360	NETL
Dilmore, Robert	Lead - Element 410	NETL
Matranga, Christopher	DOE Lead - Element 420	NETL
Klara, Julianne	Lead - Element 520, 530	NETL
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Gao, Fan	Post Doc	CMU	

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R&D FACTS

Crosscutting Research

Innovative Process Technologies

Innovative Process Technologies is concerned with the development of innovative cost-effective technologies that promote efficiency, environmental performance, availability of advanced energy systems, and the development of computational tools that shorten development timelines of advanced energy systems. NETL, working with members of the NETL-Regional University Alliance (NETL-RUA), will focus on five research tasks:

- Sensors
- Power Electronics and Energetic Materials
- Innovative Energy Concepts
- Computational Materials
- Multiphase Flow

Sensors

Better sensing of operating conditions and control strategies improves environmental performance and reduces emissions during power systems operation. Sensors and controls for process monitoring are of critical importance for advanced fossil energy applications, including oxy-fuel combustion, solid oxide fuel cells (SOFCs), advanced turbines, coal gasification, and advanced boiler systems.

Power Electronics and Energetic Materials

Application of grid scale energy storage devices will improve reliability and stability of the grid; provide capacity to “peak shave or load shift,” enabling peak loads to be met during periods when generation, transmission, and distribution assets cannot yet be brought online; enable the integration of large scale renewable energy plants into the grid; and provide more stable and efficient delivery of electrical power— including power generated from fossil fuel sources. This will result in more stable and efficient delivery of electrical power, while reducing overall CO_2 emissions.

Innovative Energy Concepts

Advanced power generation concepts such as direct power extraction, pressure-gain combustion, supercritical CO_2 cycles, and other innovative ideas have the potential to increase the efficiency and offset the penalty associated with capturing CO_2 from power generation from fossil fuels. Although these innovative energy concepts (IECs) have significant potential advantages, practical development is stymied by uncertain component performance, the need for new materials, or simply the cost of development. The goal of the IEC is to utilize validated, computational simulations that can predict performance of these IECs to identify gaps in simulations and technology and guide development and accelerate the deployment of IEC technologies.

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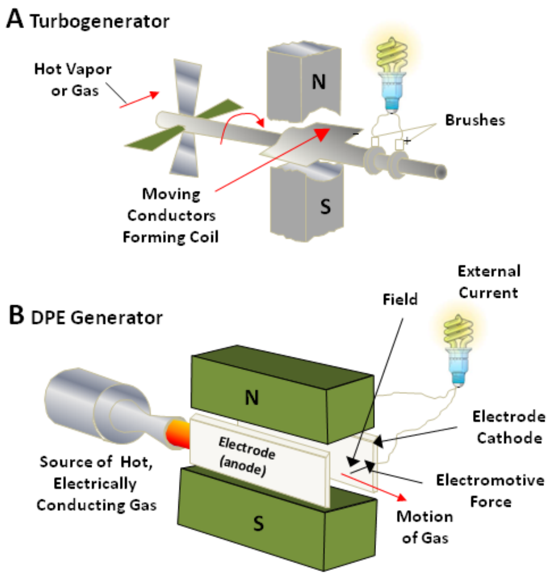
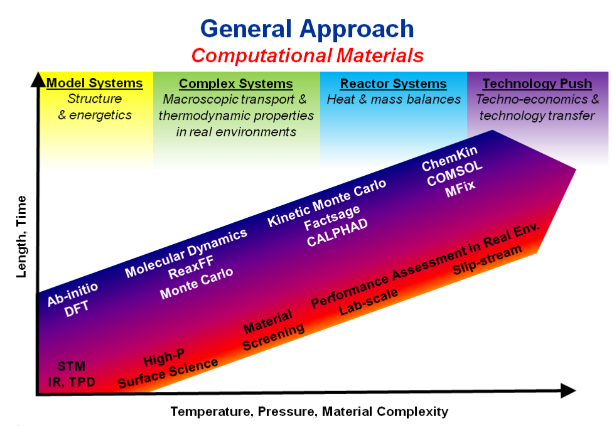


Comparison of (A) conventional power generation via a turbogenerator and (B) direct power extraction via a technique such as MDH

Computational Materials

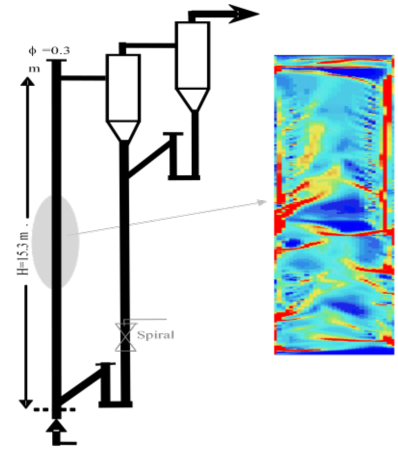
Advanced carbon capture and storage power systems will require cost-effective materials for a variety of fossil energy applications. Complex materials structures (e.g., multi-component or multi-phase materials) offer distinct advantages over single-component or single-phase materials. The properties of complex structures can be tailored or tuned by the appropriate combination and distribution of elements, constituents, or phases. However, most development efforts for complex systems are Edisonian in nature, due to the lack of predictive models and simulations for these systems. Thus, a predictive multi-scale computational framework will be fostered to guide the development of these advanced materials. The proposed effort will integrate multi-scale computational approaches with focused validation experiments. The computational tool sets developed through this research will assist in accelerating the design, development and deployment of materials for advanced Fossil Energy (FE) and other extreme environment applications.



Integrated multi-scale computational approach with focused validation experiments for accelerating the development and deployment of advanced materials

Multiphase Flow

Computational fluid dynamics (CFD) codes for multiphase reacting flows require critical research before their routine and confident employment for design and optimization. The MFIX CFD solver simulates hydrodynamics, heat transfer, and chemical reactions in fluid-solids systems. MFIX was developed at NETL to address critical aspects of fossil-fuel energy production, such as gasification or CO_2 capture. Improvements and enhancements to the MFIX solver could reduce time to solution and improve the basic understanding of polydisperse reacting flows and methodology needed to reduce data sampling for uncertainty quantification in the numerical results.

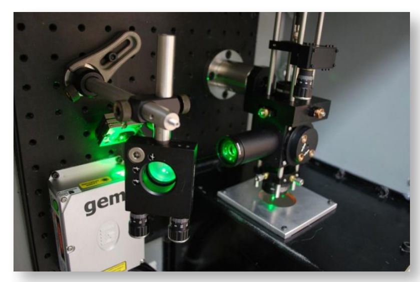


Circulating Fluidized Bed

Project Overview

Sensors

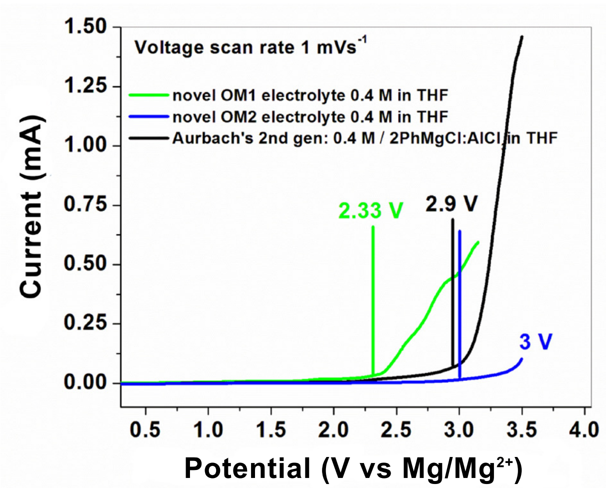
The Sensors and Controls task will develop advanced sensor materials, advanced optical sensors, and platforms (advanced materials) for high-temperature sensing, and will test novel control systems. The advanced optical sensors effort includes pre-commercial field testing, improvement of critical components, and technology transfer of a novel instrument that uses Raman scattering of a laser to measure real-time gas composition. It also includes research on using Raman scattering in a multipoint, fiber optic gas sensor. The advanced sensors materials effort is focused on synthesizing innovative thin films with a mixture of two or more different nano-scale phases having distinct electrical, optical, magnetic, and/or catalytic properties. Efforts will also focus on assessing graphene for high temperature sensor applications. The novel control system research effort will utilize the NETL Hyper facility as a platform to test novel control approaches for power generation systems, for both the MESA project with Ames Laboratory and multiple-in multiple-out (MIMO) controls.



Portable Raman Gas Composition Sensor Prototype

Power Electronics and Energetic Materials

The Power Electronics and Energetic Materials task will develop and demonstrate at laboratory scale an integrated electrochemical (anode-electrolyte-cathode) architecture with performance characteristics suitable for grid-scale power electronics and energy storage technologies. The task will continue development of a magnesium- (Mg) based battery system.



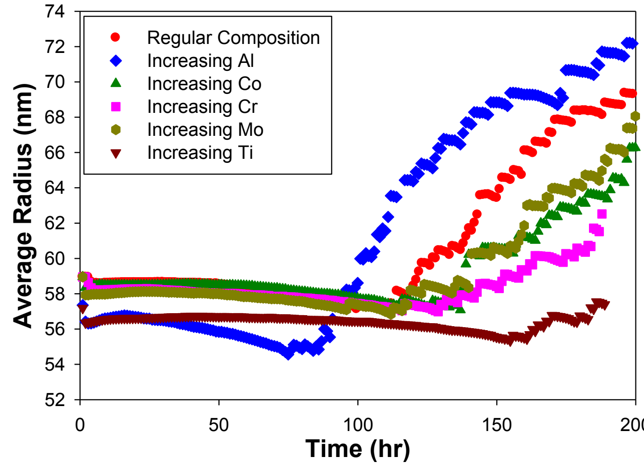
NETL-RUA Developed novel organo-metal (OM) based non-aqueous electrolyte wherein reversible Mg/Mg^{2+} deposition/dissolution observed within the electrochemical potential window of ~ 3V.

Innovative Energy Concepts

The Innovative Energy Concepts task will assess advanced concepts—magnetohydrodynamics (MHD), pressure gain combustion, and Ultra Super Critical (USC) CO_2 power cycle—using validated simulations, to accelerate the deployment of these potentially transformational systems. Advanced CFD coupled with targeted validation experiments will assess the technologies and identify gaps in simulations tools.

Computational Materials

The Computational Materials task will demonstrate a discovery and design methodology that is generally applicable to materials needed for advanced FE systems. The goal is to develop a validation computational framework that facilitates the design and development of materials by elucidating chemical and mechanical properties at conditions and time scales consistent with application. The computational tools developed through this research will assist in accelerating the design, development and deployment of materials for FE applications. Research is focused on developing computational frameworks to: (i) predict alloy oxidation behavior in a variety of relevant environments (O_2,H_2,H_2O and CO_2) - initial focus is on predicting alloy composition necessary for the formation of passive (protective) surfaces in Ni-Fe-Al alloys; (ii) predict microstructural stability – and therefore materials properties and performance – under relevant time scales for alloys under consideration for application in advanced FE systems,



Phase field simulation for microstructural evolution in alloys. This simulation is for the effect of alloying element on the coarsening of gamma prime phase in the nickel base superalloy Haynes 282.

including A-USC power plants; and (iii) aid in Electroslag Remelting (ESR) melt processing of alloys under consideration for advanced FE systems, including A-USC power plants, by establishing the thermodynamics of ESR melting and developing a thermodynamic data base for oxide and fluoride slag components used in ESR melting of Ni-alloys.

Multiphase Flow

The Multiphase Flow task seeks to develop an improved physics-based CFD capability for simulating reacting multiphase flows. This effort will focus on (i) the reduction of "time to solution" of multiphase CFD simulations through porting of NETL's open-source multiphase flow solver MFIX to graphics processing unit (GPU) architecture; (ii) improving the fidelity of multiphase CFD simulations by accounting for particle size and density distribution in reacting multiphase flows, and developing predictive capability at the porous microstructure scale of solid sorbent particles used in CO_2 capture; and (iii) including uncertainty quantification as an integral part of simulations, with incorporation of a stochastic analysis with minimal sampling technique to reduce the data sampling required.

Impacts and Benefits

The following impacts are possible through this proposed research.

- Fast optical gas composition sensor will allow engine operators to adjust control system to accommodate wide gas composition fluctuations expected in fuel flexible power generation, and gasifier operators to quickly diagnose changes in gasifier operation.

- Investigation of new materials for sensors, including nanocomposite thin films, or graphene films, may permit high-temperature gas speciation that is needed for future power plant operation, or lower cost energy harvesting for wireless sensors and other applications.

- Evaluation of advanced distributed control architectures will provide NETL and SCC a qualitative and quantitative understanding of the benefits of new distributed control methods applied to power plant operation.
- Testing of advanced sensors in the High Pressure Combustion Facility will allow DOE to push the development of new harsh environment sensors more quickly and cost effectively from laboratory research into the market.
- A novel, environmentally benign Mg-based battery architecture with performance characteristics that are potentially superior in terms of economics and performance compared to NaS and Zebra batteries for grid scale applications.
- Determination of the performance potential of innovative concepts like pressure-gain combustion and direct power extraction. Results will define the technical barriers that must be addressed to produce the desired benefits of the technology. Validation data is needed to insure that predicted performance is correct.
- Provide needed validation data on reacting flows that are relevant to current power generators, like turbines and oxy-fuel combustors, as well as future innovative technologies.
- Validated simulations will be useful to predict the behavior of current turbines, and will allow engine operators to predict/avoid combustion dynamics, flashback in hydrogen turbines, and emissions performance.
- A predictive computational framework for rapidly screening composition and configuration space for complex, multi-component materials. Computational tool sets and databanks for assessing oxidation behavior, microstructural evolution and mechanical performance of alloys in environments and times scales indicative of advanced energy systems. These tool sets and databanks will accelerate the discovery, design and development timelines for advanced materials for use in extreme environments.
- Databank of phase stability and physical properties for oxide, fluoride and mixed oxide-fluoride slags suitable refining and improving ESR melt processing.
- It is expected that the GPU acceleration of MFIX yield a 2 to 8-fold reduction in time to solution. Along with improvements in reacting gas-solid models in MFIX, the reacting multiphase ROM and reduction in the number of data sampling requirements for uncertainty quantification, the simulation capabilities put in place at the successful completion of these projects will enhance NETL's predictive capabilities to design and optimize reactors used in fossil energy systems.

NETL

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Smith, Mark	Project Lead	URS

Name	Project Role	Affiliation	University Project Title
Gellman, Andrew J Payne, Matt	PI Grad Student	CMU CMU	AlFeNi Oxidation Modeling
Bajura, Richard A	PI	WVU	CFD support of high-temperature oxy-fuel systems for magnetohydrodynamics (MHD) applications
Jaramillo, Paulina Apt, Jerome Oates, David Luke Blanco, Christian C	PI CO-PI Researcher Grad Student	CMU CMU CMU CMU	Coal Power Plant Operations in a System with Increased Wind Power
Miller, James B	PI	CMU	Combinatorial Materials Evaluation
Apt, Jerome Jaramillo, Paulina Lueken, Roger A	PI CO-PI Grad Student	CMU CMU CMU	Fossil Plan Mothball and Reactivation decisions with Increase Wind Power
Weiland, Nathan T Bedick, Clinton R	PI Researcher	WVU WVU	Fundamental Combustion Studies
Givi, Peyman	PI	Pitt	LES of Sandia Half-Scaled Dump Combustor
Vandsburger, Uri Janka, Adam	PI Grad Student	VT VT	Methods of Pulse Smoothing of Pressure Gain Combustion Events towards Enhanced Turbine Efficiency and Reliability
Gleeson, Brian M Wang, Guofeng	PI CO-PI	Pitt Pitt	Oxidation Analyses and Structure-Function Predictions for AlxNiyFe1-x-y alloys
Haworth, Daniel C	PI	PSU	PDF-Based Models for Oxy-Coal Combustion
Celik, Ismail B	PI	WVU	Simulation and Validation for Innovative Energy Concepts (S&V-IEC): WVU Combustion Modeling
Bhattacharyya, Debangsu Turton, Richard Kasule, Job Samuel	PI CO-PI Post Doc	WVU WVU WVU	Techno-Economic Optimization of Process and Energy Plants with Integrated CO2 Capture and Utilization Processes
Santavicca, Domenic A	PI	PSU	The Effect of EGR on the Performance and Operability of Lean Premixed Combustors
Boroyevich, Dushan Reed, Gregory F	PI PI	VT Pitt	The Next Generation Power Converter: Converter Topology

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R & D FACTS

Crosscutting Research

National Risk Assessment Partnership

The Need for Quantitative Risk Assessment for Carbon Utilization and Storage

Carbon utilization and storage—the injection of carbon dioxide (CO_2) into permanent underground and terrestrial storage sites—is an important part of our nation's strategy for managing CO_2 emissions. Several pilot- to intermediate-scale carbon storage projects have been performed in the U.S. and across the world. However, some hurdles still exist before carbon storage becomes a reality in the U.S. at a large scale.

From a technical point of view, carbon storage risk analysis is complicated by the fact that all geologic storage sites are not created equally. Every potential site comes with an individual set of characteristics, including type of storage formation, mineral make-up, caprock characteristics, potential natural and artificial CO_2 migration pathways, and history of tectonic activity. In addition, the characteristics of a site change over time, as do the risks associated with it. Most risks will increase or decrease with time.

Of particular relevance to making a business case for large-scale, long-term storage feasibility is the development of quantitative science-based methods for estimating long-term risks. Such methods and the tools derived from them will help address two of the more important challenges for full scale carbon storage: long-term liability and cost of monitoring, particularly for post-injection site care.

The National Risk Assessment Partnership Initiative

The National Risk Assessment Partnership (NRAP) is a DOE initiative that harnesses core capabilities developed across the National Laboratory complex, in the science-based prediction of the critical behavior of engineered-natural systems.

This core DOE capability is unique within the federal government and can support key decisions and technological solutions tied to many energy challenges, including CO_2 capture, utilization and storage (CCUS), shale-gas production, production of deepwater resources, and engineered geothermal systems.

NRAP is fostered by the National Energy Technology Laboratory (NETL) Strategic Center for Coal (SCC) and is a consortium consisting of national laboratories' research capabilities spanning DOE's Office of Fossil Energy (NETL-RUA), DOE's National Nuclear Security Administration (Lawrence Livermore National Laboratory and Los Alamos National Laboratory) and DOE's Office of Science (Lawrence Berkeley National Laboratory, and Pacific Northwest National Laboratory).

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Virginia Tech
West Virginia University

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Los Alamos National Laboratory
Pacific Northwest National Laboratory

The NRAP initiative is currently focused in support of the business case for commercial deployment of CCUS. In particular, the goal of this work is to develop defensible, science-based methodologies and platforms for quantifying risk and reducing uncertainties in order to guide decision-making and risk-management strategies that efficiently achieve DOE's goal of 99% storage permanence. NRAP will also develop monitoring and mitigation protocols to reduce uncertainty in the predicted long-term behavior of a site.

The NRAP program receives input from industry, government, non-government organizations, and academia regarding research needs for large-scale CO_2 storage deployment. The NRAP collaborative also keeps abreast of international developments by participating in collaborations like the International Energy Agency Greenhouse Gas Research and Development Programme's Risk Assessment Network.

To assist in effective site characterization, selection, operation, and management, NRAP is considering potential risks associated with key operational concerns, as well as those associated with long-term liabilities. Operational issues include the management of reservoir pressure and stress to avoid conditions that might induce seismic activity. Issues associated with long-term liabilities include groundwater protection and storage permanence to avoid CO_2 leakage.

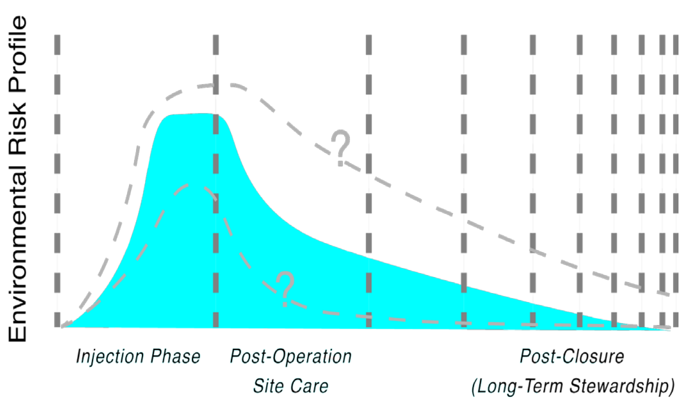

Figure 1. Risk profile curve, similar to Benson, 2004, describing the risks and associated uncertainties of a storage project over time.

NRAP Products, Expected Benefits, and Accomplishments

The NRAP project will be executed in three phases, each of which improves the science-based platform. Phase I is underway for the FY10–FY14 timeframe and focuses on quantification of risk profiles, trapping mechanisms, and associated uncertainties.

Phase II is ongoing and runs to FY15. Phase II focuses on the identification and development of risk management approaches that include strategic monitoring to verify system performance and lower uncertainty.

Phase III addresses a potential need for additional data from field test(s). An integral component of the NRAP approach is to utilize laboratory and field data to calibrate and validate models. NRAP's strategy in Phase I is to exploit existing data and ongoing field efforts to the extent possible, augmenting these data through the use of targeted laboratory-data and field-data efforts. Consequently, a Phase III field effort may be proposed for FY14 and FY15.

NRAP products for carbon utilization and storage include:

- **Simulation toolsets and protocols for quantifying storage performance and potential risks.** Primary toolsets include integrated assessment models (IAMs), supported by associated reduced-order models (ROMs). The first generation NRAP toolset was completed during FY12, and is currently being beta tested by the NRAP community. The second and third generation toolsets will add functionality and detail, as well as providing improved efficiency. Once completed and tested, these toolsets (IAMs, ROMs) will be made accessible publically through the Energy Data eXchange (EDX), with the first being made available in 2013.

- **Broadly applicable quantitative models for predicting the behavior of specific components at a storage site (such as changes in wellbore permeability due to chemical reaction).** Descriptions of the protocols and models (both detailed process models and ROMs) are being made available through the production of a publically available technical report series (TRS).

- **A web-accessible database of critical parameters for calibrating models needed to predict CO_2 storage and potential risks.** Calibration and validation data developed in the course of laboratory and field studies will be made available both through the TRS mechanism and through the EDX (as detailed datasets). First releases are expected by second quarter FY13.

- **Comprehensive technical assessments of key storage security relationships and issues.** These assessments will be made broadly available as part of the technical report series.

Expected results and benefits of NRAP's efforts include:

- Achieving the goal 99% storage retention across a range of variable factors at a storage site.
- Reducing barriers to CCUS deployment by lowering uncertainties in liability valuation studies through quantitative, science-based predictions through development of a robust methodology and platform (computational tools) for quantifying risks (and associated uncertainties).
- Guidelines and management strategies for the effective and efficient operation of storage sites (informed by a common, quantitative framework and by comprehensive technical evaluations on key issues developed by a multi-organizational team).
- Confidence in setting storage-security metrics by providing a science-based ability to identify safe operational envelopes that minimize potential risks across a range of storage environments.

The tools and improved scientific base developed by the collaborative will help operators design and apply monitoring and mitigation strategies. They will help regulators and their agents quantify risks and perform cost-benefit analyses for specific Carbon Capture and Storage (CCS) projects. Finally, financiers and regulators will be able to invest in and approve CCS projects with greater confidence because costs of long-term liability can be estimated more easily and with less uncertainty.

NRAP has completed its first generation toolset, which includes:

- First versions of integrated assessment models (and underpinning process models) for predicting potential for CO_2 release to the atmosphere, potential for CO_2 or brine impact on groundwater, and ground-motion due to fluid injection at a site.
- ROMs for brine- and gas-filled reservoir types, which were based on detailed sensitivity analyses using research and commercial simulators and based on both look-up tables and sophisticated artificial intelligence algorithms.
- Detailed process models for fluid release along a wellbore with various completion characteristics (including open wells, wells with poor cement, and wells with good cement) or along a discrete fault whose properties were predicted with coupled geomechanics simulator.

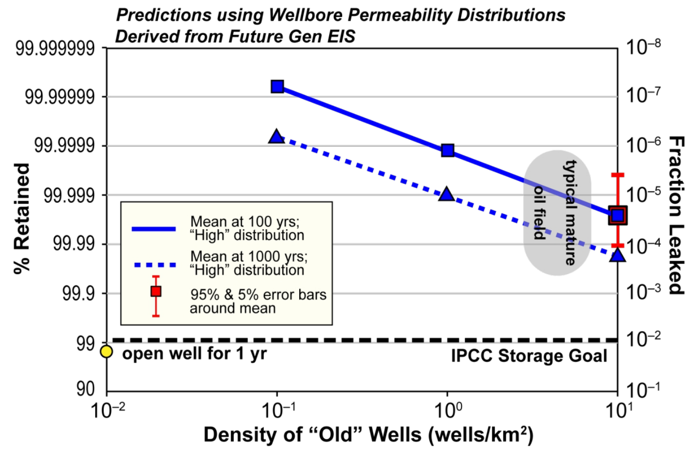

Figure 2. Preliminary results of quantitative assessment of IPCC Storage Goal of 99% retention for a particular site type.

ROMs for two end-member groundwater aquifers based on detailed hydrogeochemical simulations coupled to uncertainty-quantification software (PSUADE).

Additionally, NRAP has performed an initial quantitative analysis to address the Intergovernmental Panel on Climate Change (IPCC) goal of 99% storage retention at certain sites, and determining that the likelihood of achieving that goal is much higher than 99% at certain sites. NRAP is in the process of completing detailed, publically releasable reports on each of its products as well as providing web access to the underpinning models and calibration data to date. In addition, NRAP will be using results from the first generation to assess the accuracy and efficiency of various approaches to ROM development.

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Sams, Neal	Project Lead	URS

Name	Project Role	Affiliation	University Project Title
Dzombak, David A	PI	CMU	Acid Gas Interactions with Seal Materials under Geologic Sequestration Conditions
Nakles, David V	CO-PI	CMU	Apply An Integrated Assessment Model and Quantify Uncertainties
Small, Mitchell J	CO-PI	CMU	
Siriwardane, Hema J	PI	WVU	Develop Second Generation ROMs for Release and Transport through Seals
Mohaghegh, Shahab	PI	WVU	Develop Second Generation ROMs for Reservoir Behavior
Mohaghegh, Shahab	PI	WVU	Develop Third Generation ROMs for Reservoir Behavior
Siriwardane, Hema J	PI	WVU	Develop Third Generation ROMs for Release and Transport through Seals
Li, Li	PI	PSU	Development of a Reactive Transport Model for the Evolution of Fracture Properties under Conditions Relevant to CO2 Sequestration
Brunet, Jean-Patrick	Researcher	PSU	
Karpyn, Zuleima T	PI	PSU	Experimental Investigation of Conditions Affecting Wellbore Integrity due to Chemical Reaction Using X-ray microCT Imaging
Cao, Peilin	Grad Student	PSU	
Karamalidis, Athanasios	PI	CMU	Geochemical Effects Inter-lab Round Robin
Siriwardane, Hema J	PI	WVU	Geomechanical Response Due to a Fault Activation During Fluid Injection
Gondle, Rajkumar	Researcher	WVU	
Nambu, Hari	Grad Student	WVU	
Nakles, David V	CO-PI	CMU	Incorporate Third Generation, Reduced-Order Models into an Integrated Assessment Model
Small, Mitchell J	CO-PI	CMU	
Siriwardane, Hema J	PI	WVU	Influence of geochemical changes on Geomechanical response during CO2 Sequestration
Gondle, Rajkumar	Researcher	WVU	
Hulcher, Carter	Grad Student	WVU	
Varre, Sai Bharath	Grad Student	WVU	
Nakles, David V	CO-PI	CMU	Integrate Second Generation Reduced Order Models Into An Integrated Assessment Model
Small, Mitchell J	CO-PI	CMU	

Continued on next page

NATIONAL RISK ASSESSMENT PARTNERSHIP (NRAP) **NETL Team Technical Coordinator:** Grant Bromhal

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Small, Mitchell J	PI	CMU	Performance Evaluation and Integration of Multiple Deep Subsurface CO2 Leak Detection Monitoring Technologies
Karamalidis, Athanasios	CO-PI	CMU	
Wang, Zan	Grad Student	CMU	
Siriwardane, Hema J	PI	WVU	Prediction of seal failures during and after CO2 Injection
Nambu, Hari	CO-PI	WVU	
Varre, Sai Bharath	Grad Student	WVU	
Nakles, David V	PI	CMU	Risk assessment in CO2 geologic sequestration
Small, Mitchell J	CO-PI	CMU	
Azzolina, Nicholas	Grad Student	CMU	
Burgos, William D	PI	PSU	Utilize Observations from Analog Sites and Case Studies to Confirm Key Aspects of System Behavior and/or Methodology

the ENERGY lab

R&D FACTS

Advanced Energy Systems

Turbine Thermal Management

The gas turbine is the workhorse of power generation, and technology advances to current land-based turbines are directly linked to our country's economic and energy security. Technical advancement for any type of gas turbine generally implies better performance, greater efficiency, and extended component life. From the standpoint of cycle efficiency and durability, this suggests that a continual goal for higher gas turbine-inlet-temperatures (TITs) with reduced coolant levels is desirable.

The realization of future high-efficiency, near-zero emission turbine power systems depends on the advancement of thermal protection of hot sections, such as first-stage vanes and blades, and control of secondary flows. Current technology for protecting such airfoils relies primarily on the combined effects of a thermal barrier coating (TBC) and convective cooling. However, state-of-the-art development in both TBC materials and cooling technologies is insufficient to meet the thermal-mechanical demands imposed by hot gas with elevated turbine-inlet-temperatures. This suggests that significant advances in turbine cooling effectiveness, as well as TBC performance and durability, are required. This research effort aims to significantly advance TBC material and aerothermal cooling technologies.

Turbine Thermal Management Research at NETL

The NETL-Regional University Alliance (NETL-RUA) Turbine Thermal Management team is taking an integrated, systematic approach to addressing advanced turbine needs. The primary objective of this research is to support the hydrogen turbine technology area in meeting the DOE advanced turbine development goal, which calls for a 3–5 percent increase in power island efficiency and a 30 percent power increase above the hydrogen-fueled combined cycle baseline.

Research projects utilize the extensive expertise and facilities readily available at NETL and participating universities. The research approach includes explorative studies based on scaled models and prototype coupon tests conducted under realistic pressurized, high-temperature turbine operating conditions.

Technical goals for NETL-RUA Turbine Thermal Management research include:

- Development of novel, manufacturable internal airfoil cooling technology concepts that achieve a cooling enhancement factor of approximately five.
- Development of advanced, manufacturable airfoil film cooling concepts that achieve a 50 percent reduction in required cooling flow.
- Design, construction, and operation of a world-class facility for testing new cooling improvement strategies for the turbine rotating blade platform.

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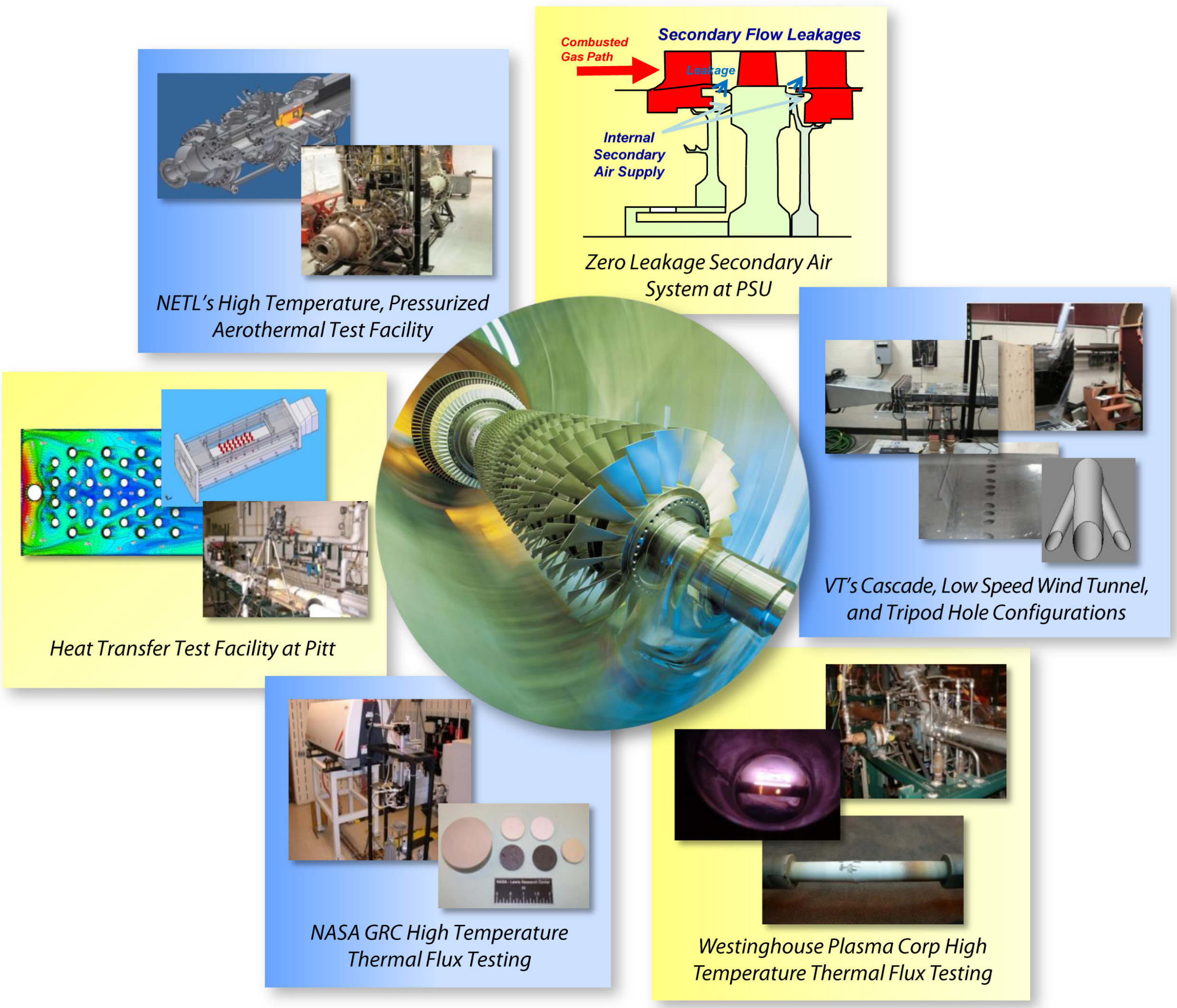
- Development of advanced material system architectures that permit operation of turbine airfoils at temperatures approximately 50–100° C higher than current state-of-the-art components.

Impact and Benefits

Research results obtained through this project can directly benefit the U.S. power and utility turbine industry by improving product development that specifically meets DOE advanced turbine program goals. Turbine technology benefited by this research will lead to products with higher efficiency and reduced emissions. Higher efficiency implies alleviating dependence on foreign oil and improving preservation of domestic natural resources. Reduced emissions will not only yield better environmental conditions but will also decrease costs for pollution controls, including carbon capture and sequestration. These factors combined will eventually lead to greater energy security and economy.



NETL's High Temperature, Pressurized Aerothermal Test Facility

Zero Leakage Secondary Air System at PSU

Heat Transfer Test Facility at Pitt

VT's Cascade, Low Speed Wind Tunnel, and Tripod Hole Configurations

NASA GRC High Temperature Thermal Flux Testing

Westinghouse Plasma Corp High Temperature Thermal Flux Testing

NETL

TURBINE THERMAL MANAGEMENT

NETL Team Technical Coordinator: Maryanne Alvin

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Richards, Geo	Focus Area Lead	NETL
Galusky, Parrish	Project Coordinator	NETL
Robey, Edward	Project Lead	URS

Name	Project Role	Affiliation	University Project Title
Gleeson, Brian M	PI	Pitt	Bond Coat and Extreme Temperature Coatings (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 3.1)
Gleeson, Brian M	PI	Pitt	Diffusion Barrier Coatings (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 3.2)
Wu, Xiaodan	Grad Student	Pitt	
Ekkad, Srinath V	PI	VT	Film Cooling (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 2.3)
Ramesh, Sridharan	Grad Student	VT	
Chyu, Minking	PI	Pitt	Internal and Transpiration Cooling (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 2.1)
Siw, Sin Chien	Post Doc	Pitt	
Miller, Nicholas R	Grad Student	Pitt	
Kang, Bruce S	PI	WVU	ODS Specifications and Preliminary Matrix Development (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 3.3.6)
Thole, Karen A	PI	PSU	Secondary Flow Rotating Rig – Facility Development (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 5.1)
Barringer, Michael	Co-PI	PSU	
Chyu, Minking	PI	Pitt	Trailing Edge Cooling (Turbine Thermal Management Field Work Proposal (FWP) Turbines-FY131415, Task 2.2)
Miller, Nicholas R	Grad Student	Pitt	

Ultra-deepwater and Frontier Regions Research Program

Assessing Risk and Mitigating Deleterious Events Associated with Drilling and Production

Background

Increasingly, offshore domestic oil and natural gas activities are associated with remote and challenging regions, such as the ultra-deepwater (greater than 5,000 feet) Gulf of Mexico and the offshore Arctic. Development in these areas poses unique technical and operational challenges, as well as distinct environmental and societal concerns. At present, ultra-deepwater resources account for approximately 32 percent of U.S. crude oil production and approximately 13 percent of total dry gas production; however, these contributions are expected to increase in the years ahead as a result of increased development activities.

Domestic resources of natural gas and oil will continue to play an increasingly critical role in meeting U.S. energy needs provided they can be produced with the confidence that environmental concerns (such as air, water, and species protection) are being addressed effectively, as noted in the President's recent executive order on the safe and responsible development of natural gas. The science base necessary to support stakeholder decisions stems from the ability to understand the behavior of engineered-natural systems over a range of often extreme conditions. NETL's Office of Research and Development (ORD) has extensive expertise in characterizing engineered natural systems associated with oil and natural gas development. This expertise is being leveraged for deepwater and ultra-deepwater hydrocarbon systems through NETL-ORD's Complementary Program in support of the Energy Policy Act (EPAct) of 2005 and in coordination with the Research Partnership to Secure Energy for America (RPSEA).

In addition to EPAct, NETL's portfolio aligns with key Federal-scale initiatives including the Ocean Energy Safety Advisory Committee (OESC), chartered February 8, 2011, to advise the Secretary of the Interior, on a variety of issues related to offshore energy safety. In particular, the findings and recommendations of the OESC's Spill Prevention Subcommittee, a multi-entity committee that seeks to address safety and potential impacts of deep offshore hydrocarbon development in the U.S. and adjoining regions, are addressed by aspects of the Complementary Program research. ORD Complementary Program research is also aligned with some of the goals of the Alaska Interagency Working Group (AIWG), led by the Department of the Interior, which brings together state, federal, and tribal government personnel to address energy-related issues and needs in the Alaskan Arctic.

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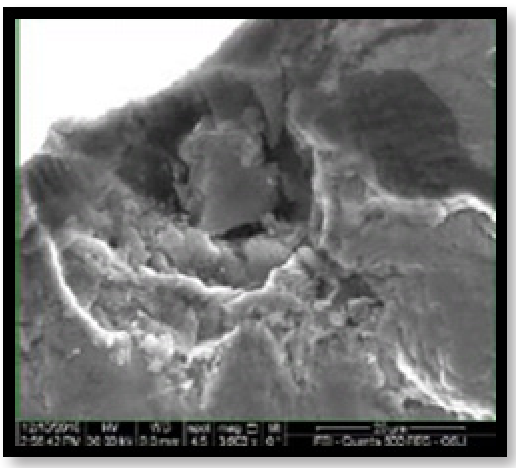
NETL Complementary Program Ultra-Deepwater/Deepwater Projects:

The objective of NETL's Ultra-deepwater and Frontier Regions research portfolio is to build the scientific understanding and assessment tools necessary to develop confidence in the safe and environmentally sustainable development of domestic oil and gas resources. The portfolio consists of six research projects that are working to address quantitative prediction of potential deleterious events in extreme offshore drilling and production. Successful implementation of portfolio research objectives will ultimately increase America's domestic oil and gas supply, reduce our nation's dependency foreign imports, and address the environmental and social concerns associated with development.

Material failures account for nearly two thirds of all loss of control events to date (SINTEF 2011), and these almost entirely align with metallic component failures and deepwater cementing issues. Three projects will broaden the Complementary Program's focus on improving the science base for key materials used in extreme drilling environments as barriers and controls, including where these materials interact in the subsurface:



Metal corrosion studies evaluate most commonly used offshore alloys

- **Characterization of Metal-Based Systems Used in Control Devices Subject to Extreme Environmental Conditions:** NETL is evaluating failure mechanisms and rates for critical components based in part on observed/reported behavior in the field augmented with experimental studies on materials behavior under simulated extreme conditions. At present, publically available data about the performance of these materials under extreme offshore conditions is limited. To date this study has successfully evaluated strength/corrosion potential the most common alloys used in extreme offshore drilling at in situ conditions (pressure, temperature, H_2S, etc). Ongoing work will result in a pit/fatigue model tool to allow for the assessment of catastrophic failure potential of these metallic components. NETL is also evaluating new alloys and surface treatments (e.g. hammer peening) for ultra-deep well environments to constrain their behavior under extreme borehole conditions.

- **Determining Physical and Chemical Behavior of Cement Barriers Used in Ultra-deepwater Systems:** NETL is researching the physical and chemical behavior of typical wellbore cements to better understand how various cement formulations perform, with a particular emphasis on potential failure pathways and remediation technologies. Currently, there is no information on how foam cements, commonly used in extreme offshore settings, perform and persist under in situ conditions. NETL researchers initiated laboratory characterization studies of commonly used industry standard formulations of foam cements and have obtained the 1st CT images of foamed cement systems. The CT characterization of the samples allows for the quantitative analysis of physical properties and structures within the cement (particularly bubble sizes and distributions). NETL researchers have also developed a reliable methodology to probe the microstructure of foamed cements under in situ conditions. Going forward, the team will use this methodology to determine stability of foamed cement systems at various "depths" in the subsurface and correlate those properties with the current method of atmospheric testing. Phase 1 findings from this project were released in a Technical Report Series (TRS) publication on NETL's website.

- **Characterization & Analysis of the Formation of Cement and Cement Casing Integrity:** A new project initiated by NETL researchers focuses on determining the physical, chemical, and temporal integrity of the formation of cement and cement casing systems used in extreme offshore settings. The project leverages NETL materials and natural systems expertise to evaluate short and long term integrity of the seal/bond between the formation, cement and casing at in situ conditions representative of the range of subsurface conditions associated with deep offshore drilling. Initially this project will focus on shallow subsurface conditions (up to 2000 feet below the seafloor) and will incorporate experimental techniques with analysis of field datasets such as borehole geophysical logs.

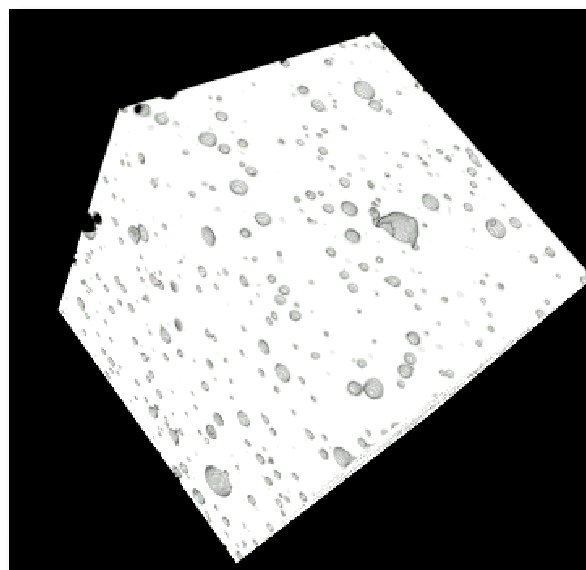
Uncertainties, such as density and viscosity, in hydrocarbon properties under in situ conditions, and behavior, such as hydrate formation and eddies, are key factors impacting the accuracy of predictions of hydrocarbon behavior and volumes both in the subsurface and in the water column during a spill event. Two projects in the offshore portfolio focus on improving the science base for multiphase fluids (like hydrocarbons, CO_2, and brine) at extreme conditions, while the final project seeks to predict, assess, and mitigate risks associated with hydrocarbon development in extreme environments in support of spill prevention and response needs:

- **Quantifying Complex Fluid-Phase Properties Under High Pressure/High Temperature (HPHT) Conditions:** NETL is working to improve the accuracy of thermodynamic models under HPHT conditions, allowing for better characterization of reservoir fluids and the dynamics of these fluids during extraction. Improved models will decrease uncertainty associated with fluid quantity and flow at and near the borehole. Accurate understanding of the reservoir and associated well behavior is an important component of our ability to predict the behavior of wells under both controlled and uncontrolled scenarios. Our lack of understanding of these extreme environments inhibits our ability to predict well behavior and develop methods for safely handling fluids under these conditions. To date, NETL researchers have expanded the density and viscosity databases for hydrocarbon compounds to span HPHT conditions. They have integrated their results with existing lower pressure and temperature data, resulting in a comprehensive database. This work is reviewed in a TRS publication on NETL's website, and an interactive database and associated application to interface with the database are under development. These will be released through NETL's Energy Data Exchange (www.edx.netl.doe.gov).

Tubulars used in offshore development

- **Improving Flow Assurance, Expediting Well Control, and Reducing Environmental Impacts Resulting from Blow-Outs in High Temperature/Low Pressure Environments:** In addition to prevention, spill response research at NETL is addressing major issues related to accurately and rapidly assessing how much hydrocarbon is leaking from a well, what is the composition of the mixture, and where does it go in the water column? NETL researchers are conducting experimental and theoretical studies to obtain fundamental, chemical, physical, and hydrodynamic information on the interactions between seawater and fluids that could be released and transported from deep, subsea hydrocarbon reservoirs and inadvertently released into a deepwater environment. This fundamental information will be used in numerical, thermodynamic, and plume models to comprehensively describe potential roles and impacts of gas hydrates. The goal of this program is to develop a comprehensive understanding of the formation and stability of simple and complex hydrates under deepwater conditions, stability of hydrates and their interaction with hydrocarbon, and the impact of dispersants, anti-agglomerants, and other chemicals used to mitigate environmental impacts on the fate and interaction of hydrates. Ultimately, the project seeks to develop a remotely-operated-vehicle (ROV) tool that can be used to rapidly and accurately determine the leak rate, composition, and fate to help guide efficient and effective spill mitigation efforts. This research is currently in the second year of a three-year effort and is on track for completion at the end of FY14.

- **Assessing Risks and the Potential for Environmental Impacts for Deepwater, Ultra-deepwater, and Frontier Regions:** Building on DOE's core competency in simulating and predicting the behavior of engineered-natural systems, NETL researchers are developing a new multi-component model tying the subsurface, wellbore and water column into a single integrated assessment modeling (IAM) tool. To effectively evaluate and reduce risks associated with extreme offshore hydrocarbon development, the IAM tool will be utilized subsurface to shore datasets which are being synthesized and integrated from a combination of existing data sources to new interpretations for the Gulf of Mexico (GOM). The targeted datasets are discussed in the recently released TRS publication on NETL's website, and an interactive database of these data layers will be released through NETL's Energy Data Exchange (www.edx.netl.doe.gov). Ultimately, this project will provide a coordinated platform (GOM IAM and EDXinsight) to allow for the independent, rapid, and science-based prediction of ultra-deepwater hydrocarbon risks and potential impacts. This will allow researchers to conduct predictive assessments of potential social, environmental, and production risk factors, and will provide recommendations on future data and technology needs to support spill prevention. The tool may also serve as a rapid-response platform in the event of future spills or deleterious events.

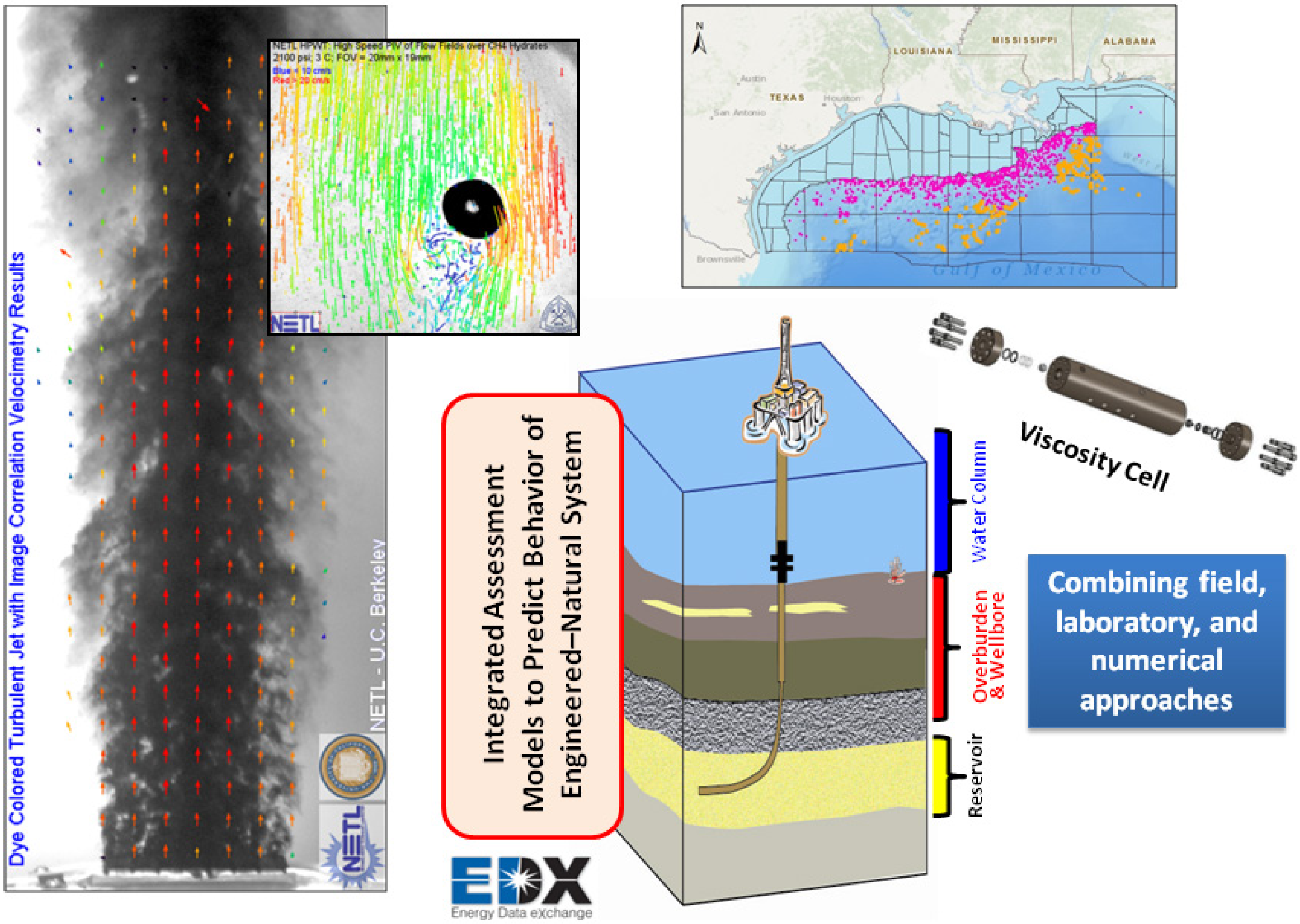


CT-image of a foam cement sample generated at NETL for bubble size distribution analysis

Find NETL TRS Publications associated with this research: www.netl.doe.gov/onsite_research/index.html

Find datasets and data-driven products associated with this research: Energy Data Exchange www.netl.doe.gov

Research to Support Science-Based Decision Making for Spill Prevention & Response



R&D 165, February 2013

ULTRA-DEEPWATER AND FRONTIER REGIONS RESEARCH

NETL Team Technical Coordinator: Kelly Rose

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Morreale, Bryan	General Eng	NETL
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Bromhal, Grant	General Eng	NETL
Crandall, Dustin	Project Lead	URS
Gill, Magdelena	Scientist	URS

Name	Project Role	Affiliation	University Project Title
Enick, Robert Baled, Hseen	PI Post Doc	Pitt Pitt	Equation of State Model Assessment and development
Enick, Robert Baled, Hseen	PI Post Doc	Pitt Pitt	Evaluate Heavy Oil Viscosity Standard
Liu, Xingbo Chen, Ting	PI Graduate Student	WVU WVU	Experimental and numerical evaluation of key metal-based failures
Enick, Robert Baled, Hseen Xing, Dazun Baled, Hseen	PI Post Doc Post Doc Grad Student	Pitt Pitt Pitt Pitt	Quantifying complex fluid-phase properties at high pressure/high temperature (HTHP)
Anderson, Brian Velaga, Srinath	PI Grad Student	WVU WVU	Plume Modeling for High-pressure Water Tunnel Facility

the ENERGY lab

R&D FACTS

EPAct Complementary Program

Unconventional Energy Resources

Background

Natural gas and crude oil provide two-thirds of our Nation's primary energy supply and will continue to do so for at least the next several decades, as the Nation transitions to a more sustainable energy future. The natural gas resource estimated to exist within the United States has expanded significantly, but because this resource is increasingly harder to locate and produce, new technologies are required to extract it.

Under the Energy Policy Act of 2005, the National Energy Technology Laboratory is charged with developing a complementary research program supportive of improving safety and minimizing the environmental impacts of activities related to unconventional natural gas and other petroleum resource exploration and production technology (EPAct 2005, Sec. 999A). This area aligns with the recommendations put forward in the SEAB Federal Research Report on Shale Gas, and efforts amongst Federal agencies to coordinate unconventional oil and gas research (unconventional.energy.gov).

The Energy Policy Act of 2005 Section 999 Complementary R&D Program is being performed by NETL's Office of Research and Development. In the area of unconventional energy resources, research is focused on developing a predictive capability to interpret how the engineered-natural systems that are developed to extract unconventional energy resources behave under various scenarios. The resulting data sets and modeling tools will provide a robust foundation for scientifically-based regulatory decision making and public knowledge.

Goals and Objectives

Unconventional energy resources research through NETL's Office of Research and Development (ORD) is focused on developing the data and modeling tools needed to predict and quantify potential risks associated with oil and gas resources in shale reservoirs that require hydraulic fracturing or other engineering measures to produce. The major areas of focus include:

- Improving estimates of fugitive methane and greenhouse gas emissions;
- Predicting the composition and volumes of water produced during shale gas development;
- Predicting subsurface fluid and gas migration, and
- Evaluating fracture growth and ground motion due to oil and gas operations.

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This project is part of the DOE/NETL Complementary Research Program under Subtitle J, Section 999 of the Energy Policy Act of 2005.

U.S. DEPARTMENT OF ENERGY

The above research areas require a combination of field monitoring, laboratory experimental and characterization, data mining, and modeling activities, and are being performed by an interdisciplinary team comprised of Federal, contractor, and academic scientists and engineers through the NETL Regional University Alliance.

Project Descriptions

Fugitive Air Emissions and Greenhouse Gases:

NETL efforts focus on improving fugitive emissions factor calculations and field emissions data sets for natural gas operations. The large uncertainty in the emissions factor used for upstream greenhouse gas emissions is being addressed through research to develop an improved method for calculating shale gas greenhouse gas emissions factors that can be applied to various shale gas basins. The limited number of high-quality field data sets representative of shale gas operations is being addressed through collection of field measurements to evaluate both ambient (regional effects) and point-source (specific process component) air emissions, with a focus on the Appalachian Basin for current efforts. Updated emissions factors based on the DOE methodology, and field data from Appalachian Basin monitoring, will reduce uncertainties in the NETL shale gas greenhouse gas life cycle assessment.

NETL's air quality monitoring trailer collecting measurements during active hydraulic fracturing

Produced Water Management:

NETL efforts focus on improving knowledge of produced water volumes and compositions, and influences of different treatment processes on management of produced liquid and solid wastes. The treatment and disposal (or reuse) of produced water is a major issue for hydraulically-fractured shale reservoirs, and is being addressed through developing an understanding of how chemical, biological, and physical factors affect produced water composition under different scenarios. Solid wastes, such as drill cuttings and water treatment residues, need to be disposed of appropriately in order to avoid environmental issues, and NETL is performing laboratory experiments to evaluate the potential for contaminant release from solid wastes under different environmental scenarios. The limited ability to predict the volumes and composition of produced waters from shale gas operations is being addressed through development of a systems-level predictive model for estimating the volumes and composition of produced waters for a shale gas basin.

NETL researcher takes water sample

Subsurface Migration of Gas and Fluids:

NETL efforts focus on an ability to evaluate the influence of wellbores and natural pathways on gas and fluid leakage, and the development of specific tracer tools to track gas and fluid migration in the subsurface. NETL is developing rapid sample processing and analytical chemistry tools for natural geochemical tracers that can be used to identify the sources of fluids and gases in complex geologic systems undergoing energy development. Existing wellbores (that may serve as conduits for fluid and gas migration from depth to shallow systems) are being identified through field magnetic surveys coupled with data mining to evaluate densities and locations of potential leakage pathways. NETL is performing laboratory work to investigate the effect of gas on well cements, and also is performing research to evaluate the effect of drilling on shallow gas distribution in groundwaters.

Predicting Fracture Growth and Ground Motion:

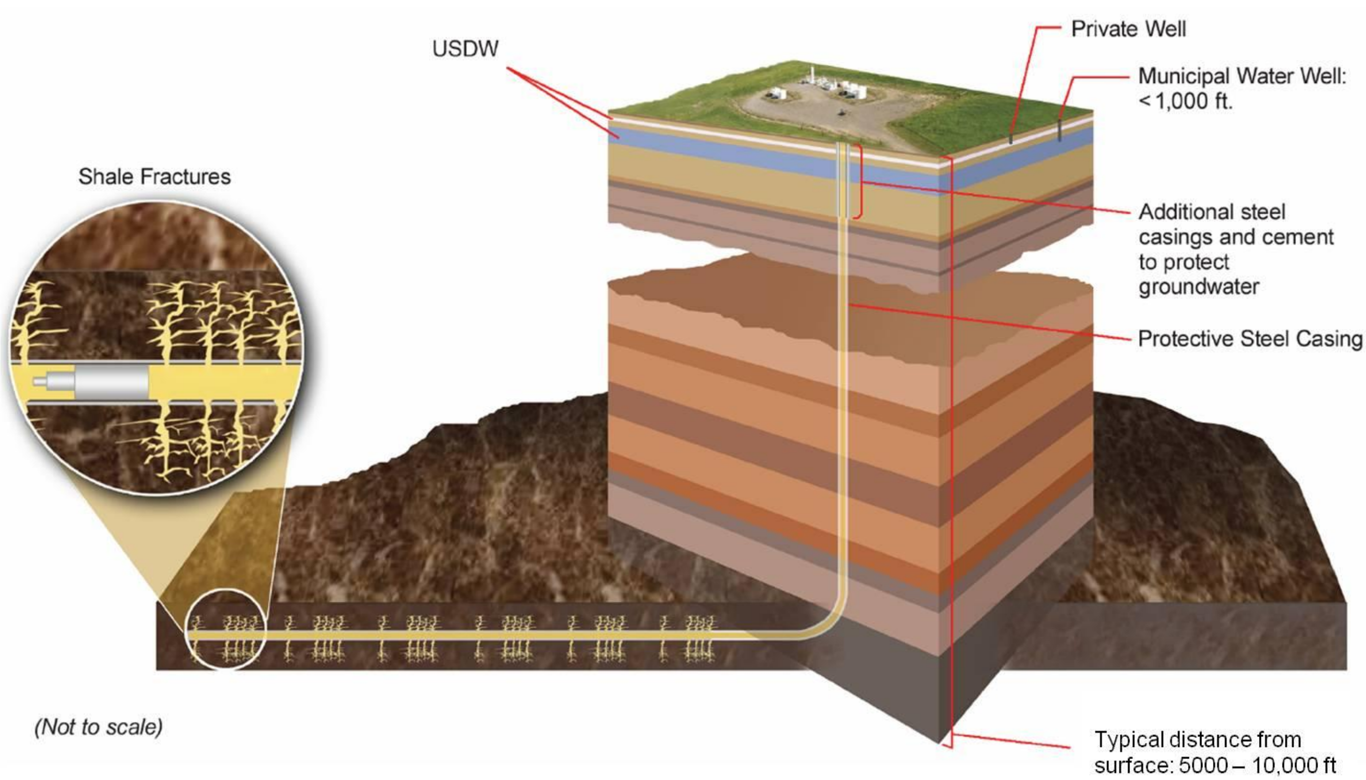
NETL efforts focus on evaluating implications of fracture growth during hydraulic fracturing, and induced seismicity related to unconventional oil and gas development. Our current ability to verify the extent of fracture growth out-of-zone remains limited, and NETL is using existing commercial software to develop fracture models that represent vertical and horizontal extents of fractures outside of the target zone, validated by field microseismic data. This information will be used to evaluate whether new fractures can intersect with other leakage pathways to the surface (such as existing wellbores). NETL also is evaluating the science base behind observed induced seismic events due to oil and gas-related activities.

Benefits

- Unbiased information to policymakers and the public.
- Objective baselines established for Marcellus shale environmental monitoring.
  - Near-term and long-term impacts documented.
  - Inventory of emissions.
  - Data sets that detail the composition of fluids produced during hydraulic fracturing.
  - Models of subsurface systems.
- New tools that allow rapid predictions of possible safety and environmental impacts associated with unexpected events.
- Quantitative assessments that characterize geologic system behavior.
- New tools for predicting the behavior of the geologic system during shale gas development.
- Optimized production from tight gas formations, shales, coalbeds, hydrates, and more.

Recent Accomplishments

- NETL's models (verified with field-based microseismic measurements) have demonstrated the infeasibility of hydraulic fractures extending to drinking water aquifers for most places in the Marcellus Shale and several other shale formations. These validated/calibrated models are being used to predict the possibility of release of gases through combined fracture/wellbore pathways.
- NETL's methodology for calculating emissions factors for methane release during upstream shale gas activities is in the final stages of development, and the new value will be used to update the NETL shale gas greenhouse gas life cycle analysis.
- NETL developed a rapid-throughput analysis technique for analyzing natural tracers as indicators of fluid leakage from shale gas systems (strontium isotopes). These techniques decrease sample processing and analysis time by an order of magnitude (one day versus one week to process a sample set). The method is currently undergoing external peer review.



Schematic of hydraulically-fractured shale gas system

R&D 166, February 2013

UNCONVENTIONAL ENERGY RESOURCES **NETL Team Technical Coordinator:** Alexandra Hakala

Name	Title	Affiliation
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Peckney, Natalie	General Eng	NETL
Veloski, Garret	Research Chemist	NETL
Diehl, Rod	Physical Scientist	NETL
Hammack, Richard	Physical Scientist	NETL
Wells, Art	Research Chemist	NETL
Stanko, Denny	Phy Sci Tech	NETL
Hedges, Sheila	Research Chemist	NETL
Lopano, Christina	Physical Scientist	NETL
Edenborn, Harry	Microbiologist	NETL
Goodman, Angela	Physical Scientist	NETL
McIntyre, Dustin	Mechanical Eng	NETL
Soeder, Daniel	Physical Scientist	NETL
Mroz, Thomas	Geologist	NETL
Strazisar, Brian	Physical Scientist	NETL
Kutchko, Barbara	Physical Scientist	NETL
Rose, Kelly	Geologist	NETL
Brohmal, Grant	General Eng	NETL
McIntyre, Dustin	Mechanical Eng	NETL
Seol, Yongkoo	Physical Scientist	NETL
Siegel, Joel	Project Lead	URS
Murin, Tim	Research Scientist	URS
Jain, Jinesh	Research Scientist	URS

Name	Project Role	Affilation	University Project Title
Glosser, Deb Bain, Daniel	Grad Student PI	Pitt Pitt	Characterizing Density and Distribution of Legacy Wells w ithin the Aerial Extent of Shale Gas Plays for Integrated Assessment of Risk
Boardman, Gregory Countess, Stephanie Sharma, Shekar	PI Grad Student Grad Student	VT VT VT	Chemical characterization of produced w ater sludge
Wood, Petra B Davis, Ryan Sheehan, James	PI Grad Student Grad Student	WVU WVU WVU	Environmental characterization (avian) prior to and during site w ell-pad construction and drilling
Capo, Rosemary C Stew art, Brian W	CO-PI CO-PI	Pitt Pitt	Evaluate isotopic composition of geologic end-members and fluid samples (Capo – Stew art Pitt)
Gregory, Kelvin B Mohan, Arvind	PI Grad Student	CMU CMU	Fate of naturally occurring radioactive material (NORM) in flow back and produced w aters from shale gas development sites (Gregory – CMU)
Vidic, Radisav D	PI	Pitt	Fate of Naturally Occurring Radioactive Material (NORM) in Flow back and Produced Waters from Shale Gas Development Sites (Vidic – Pitt)
Iannacchione, Anthony Vandenbossche, Julie	CO-PI CO-PI	Pitt Pitt	Gas flow from shallow gas formations
Li, Li	PI	PSU	Geochemical modeling - integration of isotope signatures
Karamalidis, Athanasios Noack, Clint	PI Grad Student	CMU CMU	ICP-MS measurement of rare-earth elements in brines
Zorn, Erich Harbert, William	Grad Student PI	Pitt Pitt	Induced seismicity monitoring using an array of geophones at an Industry host site
Small, Mitchell	PI	CMU	Integrating Atmospheric Dispersion Models and Statistical Analysis of Monitoring Data to Identify Leakage at Shale Gas Sites
Siriw ardane, Hema	PI	WVU	Model simulation of rock failure due to long term fluid injection
Westman, Erik	PI	VT	Physics-based geomechanics, rock properties, and modeling to predict fracturing of shale
Wang, John Yilin	PI	PSU	Predicting volumes and compositions of produced w ater
Siriw ardane, Hema	PI	WVU	Prediction of Fracture propagation in a multi-layered geologic formation
Karamalidis, Athanasios	PI	CMU	Shale-fluid interactions that lead to metal release
Sharma, Shikha Bow man, Lindsey Warrier, Ajaya	PI Grad Student Technician	WVU WVU WVU	Stable Isotopes as Indicators of Fluid Sources and Fluid-Rock Interactions in Complex Geological Systems

Continued on next page

UNCONVENTIONAL ENERGY RESOURCES **NETL Team Technical Coordinator:** Alexandra Hakala

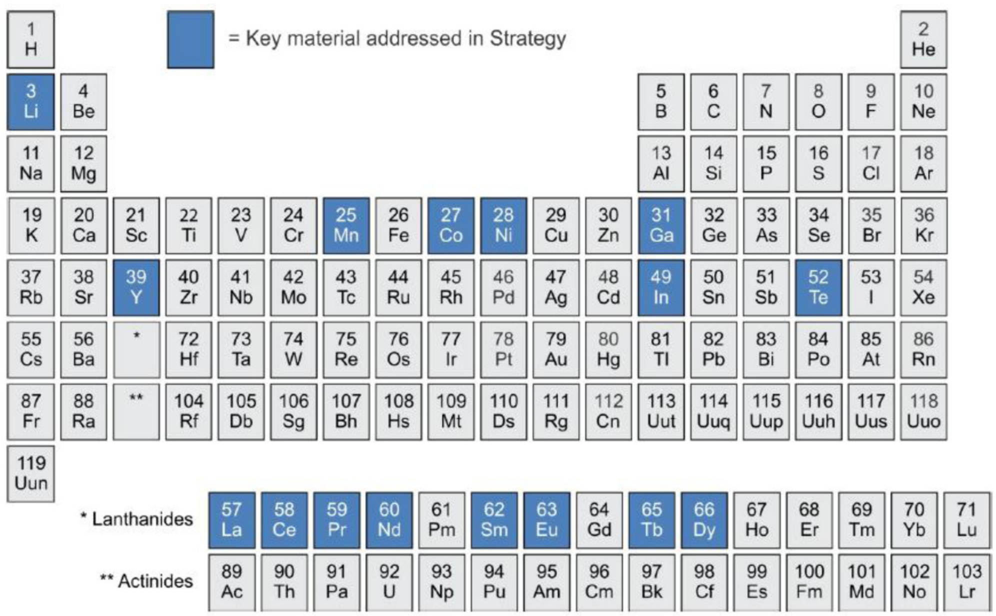
Name	Project Role	Affilation	University Project Title
Siriwardane, Hema J	PI	WVU	Coupled Thermal-Hydrological-Geomechanical Modeling of Gas Hydrates to Support Field Tests
Lin, Jeen-Shang	PI	Pitt	Geomechanical Strength, Deformability and Seismic Properties of Hydrate Bearing Sediments and Numerical Analysis - Constitutive Model Development
Sharma, Shikha Yao, Jianbo	PI PI	WVU WVU	Integrated Chemo-stratigraphic Characterization and Biogenic Stimulation of Organic Shale
Anderson, Brian McGuire, Patrick Sridhara, Prathyusha Anderson, Brian McGuire, Patrick Garapati, Nagasree	PI Researcher Grad Student PI Researcher Grad Student	WVU WVU WVU WVU WVU WVU	Numerical Reservoir Simulations for Gas Production Field Tests - BP Field Test Simulation Support
Capo, Rosemary C Stewart, Brian W Phan, Thong Thai Kolesar, Courtney Achille, Megan	CO-PI CO-PI Post Doc Grad Student Under Grad	Pitt Pitt Pitt Pitt Pitt	Optimizing parameters for predicting the geochemical behavior and performance of discrete fracture networks in geothermal systems
Li, Li Brunet, Jean-Patrick Wen, Hang	PI Researcher Researcher	PSU PSU PSU	Optimizing parameters for predicting the geochemical behavior and performance of discrete fracture networks in geothermal systems
Sharma, Shikha Henry, Stephen J Warrier, Ajaya	PI Grad Student Technician	WVU WVU WVU	Optimizing parameters for predicting the geochemical behavior and performance of discrete fracture networks in geothermal systems
Anderson, Brian McGuire, Patrick Gaddipati, Manohar	PI Researcher Grad Student	WVU WVU WVU	United States Geological Survey (USGS) Alaska North Slope Gas Hydrate Development Life Cycle Assessment

The Critical Materials Research Alliance

About the Critical Materials Research Alliance

The recent surge of interest in critical materials, including rare earth elements (REEs), stems from supply shortages and escalating prices of some REEs. In 2010, the United States' sole REE supplier was China—previously responsible for 97% of global REE production—but the Chinese government curtailed their export. Because REEs and other critical elements are used in renewable energy resources, energy storage, energy efficiency technologies, and national defense, a shortage in their supply impedes development of energy technologies and hinders U.S. defense industries.

To address the challenges faced in revitalizing the rare earth industry, the National Energy Technology Laboratory (NETL) and several prominent research institutions and industrial partners[1] have collaborated to form the Critical Materials Research Alliance (CMRA). World-renowned researchers associated with CMRA work with a range of extraction and materials technologies and research novel ways to use critical materials in the energy industry, while industrial partners either produce elements critical to energy technologies or use those elements to produce components for advanced technologies.



Key Materials

NETL and its partners work collaboratively, so all involved parties can access expertise and specialized facilities at other member institutions, thereby making a broader range of in-depth research possible. The variety of research institutions will also allow future scientists greater choice in study locations and disciplines of study.

1 University partners in NETL-RUA are the Carnegie Mellon University (CMU), Pennsylvania State University (PSU), University of Pittsburgh (Pitt), Virginia Tech (VT), and West Virginia University (WVU). The URS Corporation is also an NETL-RUA partner institution.

Primary Activities of CMRA

CMRA performs research to identify and tackle the technological challenges associated with revitalizing domestic industries and increasing their competitiveness in areas related to critical materials—such as lanthanides (rare earths) and other elements that our nation largely imports—and the applications in which they are considered vital.

REEs are already used in the manufacture of generators for windmills, electric and hybrid vehicles, next-generation batteries, light emitting diodes (LED), compact fluorescent lights (CFL), solar panels, catalysts for oil refining, solid oxide fuel cells, and auto exhaust conversion. For defense, REEs appear in various sensors used for cruise missiles, smart bombs, drones, sonar transducers for submarines, radars, and tanks. Development of REEs in response to the shortage mentioned will allow their continued use and the possibility of other applications.

	Photovoltaic Films	Wind Turbines	Vehicles		Lighting
MATERIAL	*Coatings*	*Magnets*	*Magnets*	*Batteries*	*Phosphors*
Indium	●				
Gallium	●				
Tellurium	●				
Dysprosium		●	●		
Praesodymium		●	●	●	
Neodymium		●	●	●	
Lanthanum				●	●
Cobalt				●	
Manganese				●	
Nickel				●	
Lithium				●	
Cerium				●	●
Terbium					●
Europium					●
Yttrium					●

Applications

CMRA intends to—

- **Develop technologies to enable the exploitation of diverse supply sources.** These include extraction technologies for minerals that have not been subject to previous commercial efforts and the development of separation technologies for high-volume byproduct and waste streams that contain large total quantities of critical elements, albeit in low concentrations.

	MATERIAL	*Nuclear Power*	*Grid Storage*	*Vehicle Light-weighting*	*Magnetic Refrigeration*	*Gas Turbines*	*Fuel Cells*	*Catalytic Converters*
Key Materials	Indium	●						
	Dysprosium				●			
	Praesodymium				●			
	Neodymium				●			
	Lanthanum						●	
	Cobalt	●					●	
	Cerium						●	●
	Yttrium					●	●	
Materials to Watch	Magnesium			●				
	Vanadium		●					
	Gadolinium	●						

Materials to Watch

- **Develop a portfolio of viable technologies.** To support the reinvigoration of domestic industry and U.S. technological competitiveness, the scope of investigations will cover a spectrum of challenges from extraction to usable commodity and a full range of critical applications.

- **Perform research at all stages of technology advancement—from basic science to applied science, development to deployment.** New insights in basic science are the catalyst for groundbreaking technologies, and development and deployment activities are necessary to turn those insights into commercially useful products.

- **Develop flexibility for key technologies.** CMRA will develop advanced/high-performance materials that use critical elements more efficiently, use less of them, or even avoid their use altogether. CMRA will also develop materials that allow us to bypass high-performance materials in novel technologies.

- **Emphasize commercialization.** To improve our economic, energy, and national securities and to ensure the technological competitiveness of our industries, the challenges that face everything from extraction to applications must be addressed. Industry must have a strong presence in research, from conception onward. CMRA research activities are vertically integrated to promote investment.

Rare Earth Oxides

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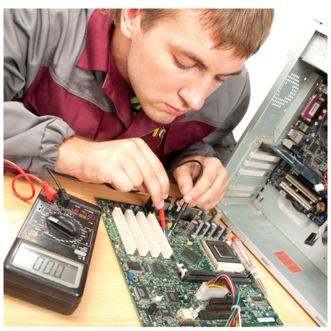
CMRA Mission and Goals

CMRA's goals for the collaborative include—

- Increasing the nation's supply of critical materials by developing the technologies needed to extract these elements from untapped, and often unconventional, domestic sources.
- Increasing the nation's flexibility in meeting demands for high performance materials by developing alternate materials and technologies that do not require high quantities of critical materials.
- By conducting quality research and training personnel, develop an intellectual infrastructure to support the revitalization of domestic industry and advance our technological competitiveness.
- Providing unbiased, complete information to industry and policy makers through an interdisciplinary review of materials, technologies, and economic, environmental, and policy considerations.

NETL-RUA
Regional University Alliance



The NETL-RUA Grid Technologies Collaborative

About the Grid Technologies Collaborative

The Grid Technologies Collaborative (GTC) is an industry-university-government integrated research and development group that advances the state-of-the-art in transmission and distribution system level power electronics technologies. Participants in the collaborative include industry partners and researchers from the U.S. Department of Energy's National Energy Technology Laboratory Regional University Alliance (NETL-RUA)[1] and the University Energy Partnership (UEP).[2] The GTC executes a comprehensive program of fundamental research; technology development, simulation and modeling, testing, and commercialization; and professional training for the advanced grid technologies sector.

Primary Activities of the GTC

The GTC engages in three primary activities:

- Developing new grid-scale power electronics devices for emerging AC and DC electrical infrastructure, supporting systems and algorithms, and demonstrating their economic value.
- Educating the next generation of power electronics engineers through advanced curriculum at member universities and training programs for existing professionals.
- Partnering with industry and the public sector to advance the technology and demonstrate benefits of advanced power electronics through collaborative research and development, seminars, and workshops.

[1] University partners in the NETL-RUA are: the University of Pittsburgh (Pitt), Carnegie Mellon University (CMU), West Virginia University (WVU), Pennsylvania State University (PSU), and Virginia Polytechnic Institute (VT). The URS Corporation is also an NETL-RUA partner institution.

[2] The University Energy Partnership (UEP) serves as a non-profit support organization and constituency liaison for the development of key NETL-RUA initiatives.

GTC Mission and Goals

The U.S. electricity transmission system—the Grid—is in desperate need of expansion and updating. Much of the basic design and main infrastructure of the grid is over 50 to 100 years old in most parts of the U.S. Improving the performance of the grid is a key component to improving energy efficiency, reliability, and power security; as well as for integrating a balanced clean-energy resource portfolio. There have been considerable efforts devoted to developing and deploying technologies for "smart grids"—a collection of technologies enabling better point-of-use control of electricity, typically at the end-use level of the system. Comparatively little attention has been focused on advancing key utility-scale transmission and distribution system technologies.

Advanced power electronics are at the core of improving the performance of the grid. Power electronics are devices and systems that facilitate the delivery of electricity from generators to end users. The power supply that many of us carry to power our laptop is a power electronics system. When deployed on the grid, as they have been for four decades, advanced power electronics systems provide four primary benefits:

- *Mitigating the need to build new transmission capacity*. By dynamically compensating for constraints in the grid, power electronics systems can maximize the flow of real power through the transmission system. This increases the amount of electricity delivered to consumers and helps to forestall expansions of the system. Power electronics are the key enabler of High-Voltage Direct Current (HVDC) transmission systems, which have higher capacities than comparable alternative current systems and can further assist in controlling the flow of electricity through the grid. In addition to core power transmission delivery applications, configurations for Back-to-Back DC links can provide greater power system security and control between major AC control networks and for interconnecting asynchronous systems.

- *Supporting liberalized electricity markets*. Prior to the arrival of liberalized electricity markets, system operators would control flows of power and system voltages by turning on and off generating assets and through mechanical switching of AC components, as needed. Today, to carry out these duties, system operators must be able to control dynamically the flow of electricity through the system and maintain proper voltage profile. Flexible Alternating Current Transmission Systems (FACTS) can control the impedance of the transmission system, giving system operators more control over how electricity flows from generators to users, as well as providing dynamic VAR regulation for voltage control and power system stabilization.

- *Integrating renewable generating resources*. There are mandates throughout the United States to produce more electricity from renewable resources, specifically solar and wind. However, the output of these systems can be highly variable, consume significant amounts of reactive power, and can result in voltage and system instability concerns. Power electronics systems—the form of both AC and DC applications—can help to mitigate these effects, facilitating the contribution of these resources to U.S. electricity generation. Power electronics systems will become even more essential as renewable resources increase their penetration into the grid, including both on-shore and off-shore resources.

- *Increasing power system stability, security, and reliability*. To properly support economic activity the grid must deliver high quality electricity—electricity that conforms tightly to voltage and frequency specifications—that is also highly reliable. However, a system operating near its capacity limits and supporting increased generation from renewable resources—which are smaller and less reliable—would seem to run counter this need. Power electronics systems are central to addressing these concerns; so much so that they are now considered an essential component of any project to expand transmission capacity and support the operations of the existing system.

Given the benefits provided by grid-scale power electronics and the clear regional, national, and international need for advances in these systems, the NETL-RUA formed the GTC. Through its activities, the GTC performs research and development across the core technologies underlying advanced power electronics. Areas of investigation include:

- *Modeling, simulation, and analysis*
- *Power semiconductors and materials development*
- *Circuit and device design, integration, and topologies*
- *Advanced control, systems interface, and protection*
- *Testing and turnkey systems integration*
- *Deployment and operations*

To further the commercialization of technologies developed by the GTC, it works closely with industry, building off the established relationships of the partner universities and engaging all relevant constituents engaged in the chain of power electronics development and applications. Industry partners bring real-world perspective to the research and development activities of the GTC. For example, GTC partner URS currently manages more than $4 billion in transmission and distribution investment projects worldwide, about half of which is for grid upgrades in which power electronics are applicable. Moreover, the GTC provides key educational initiatives and staff development services for its industrial partners.

GTC Vision

An advanced electricity transmission and distribution network that is operationally efficient and highly reliable; facilitates the integration of renewable and distributed generating supplies, and energy storage systems; is resilient to disruptions; and provides the most appropriate form of electricity to advance economic development.

The GTC achieves its vision by performing R&D on power electronics technologies for transmission and distribution system applications, including device development, integration, modeling and simulation, control, and fundamental research on key enabling and disruptive technologies. Through its industrial partners and government sponsors, the GTC facilitates the deployment of power electronics systems and helps to educate the next generation of electric power system and power electronics professionals.

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NETL-RUA
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U.S. DEPARTMENT OF ENERGY

R&D FACTS

Strategic Growth Area

Shale Energy Resources Alliance (SERA)

Mission

To support the environmentally and socially sustainable development of shale resources through collaborative research and development among industry, university, and government partners on: resource characterization; drilling and extraction technology; near-term and cumulative environmental and social impacts; and empirically supported policy.

To achieve this mission, SERA conducts research on key areas related to shale energy development, develops and demonstrates technologies supporting the environmentally sustainable development of shale energy resources, serves as a repository of data regarding shale energy resources and environmental effects, and promotes dialogue among stakeholders.

Vision

A world in which global supplies of shale resources are developed economically, while promoting environmental sustainability.

An NETL-RUA researcher filters a water sample from drilling site.

A produced water pond at one of the NETL-RUA's industry partner sites.

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NETL-RUA PARTNERS

Carnegie Mellon University
Penn State
University of Pittsburgh
URS Corporation
Virginia Tech
West Virginia University

Key Activities

SERA realizes its mission through the following core activities:

- Advancing the fundamental science of shale gas resources and extraction, focusing on air quality, water resources (sources, effects on, and treatment and disposal of produced water), and geology;
- Developing and demonstrating advanced technologies to support environmentally sustainable shale gas production;
- Serving as a repository of data for activities related to shale gas exploration; development, and effects while publishing peer-reviewed research based on those data; and
- Promoting information exchange among shale gas producers and suppliers, researchers, non-governmental organizations, and the public.

Overview of Planned Research

Air Emissions

Research in this area will advance the state of the art in regional air quality modeling and lifecycle greenhouse gas (GHG) assessment as it relates to the development of shale gas resources. The results will: (1) provide a basis for local, regional, state, and federal decision makers to take positive actions to improve air quality; (2) identify opportunities for technology to reduce emissions from shale gas development and operations; and (3) provide a scientific basis for estimating the potential reductions in GHGs from employing shale gas resources.

Water – Sourcing and Disposal

This research seeks to establish SERA as a single resource that evaluates the costs and performance of the various water management options for the shale energy sector. Water resources to support development of shale gas resources can be constrained. Costs related to various treatment options range from manageable to exorbitant and can seriously affect the economics of a given well. While many treatment technologies are available on the market, there are many that are unproven in the shale gas context. Finally, the effect of shale gas development on regional hydrogeology is an area of key interest.

Shallow Stray Gas

Shallow stray gas in the Marcellus formation has been a common safety concern for many stakeholders. Potential sources of the gas include operating or abandoned gas wells, active or inactive deep mines, permitted or un-permitted landfills, natural gas pipelines, or microbial gas generated in the shallow subsurface. This research supports the NETL-RUA Shale Gas SGA program goals and objectives by evaluating whether naturally forming gas can affect groundwater aquifers, determining the extent and magnitude of gas migration along wellbores, and providing solutions to prevent gas flow in the wellbore from shallow gas formations.

An NETL-RUA researcher samples groundwater at a Marcellus site.

Boom-mounted magnetometers identifying abandoned wells for drilling companies.

NETL's mobile air monitoring laboratory at shale drill site in the Marcellus formation.

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U.S. DEPARTMENT OF ENERGY

R&D FACTS

Strategic Growth Area

NETL's Simulation-Based Engineering User Center

Introduction

The National Energy Technology Laboratory (NETL) is home to the Simulation-Based Engineering User Center (SBEUC), which hosts one of the world's largest high-performance computers along with advanced visualization centers serving the organization's research and development needs.

A unique and collaborative tool tailored for engineering calculations in support of fossil energy research, the SBEUC progresses NETL's mission by applying complex model simulations for advanced energy technology development; simulations like these will help overcome technical barriers in development quickly, reliably, and cost-efficiently.

The NETL teams responsible for designing the SBEUC have balanced computational requirements, efficiency, usability, and collaboration techniques to deliver a premier system to the Lab and its partners.

Computational Capabilities

At the heart of the SBEUC is the HPCEE, or High-Performance Computer for Energy and the Environment, a 503 TFlops (trillion floating-point operations per second) high-performance computer that enables the simulation of phenomena that are difficult or impossible to measure, such as coal jet penetration into a gasifier.

The Center also has capabilities for running modeling tools at various scales ranging from molecules, to devices, to entire power plants and natural fuel reservoirs. With these capabilities the SBEUC provides enhanced visualization, data analysis, and data storage capabilities that enable researchers to discover new materials, optimize designs, and predict operational characteristics.

Pictured are the computational nodes inside of modular datacenter.

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Penn State University

University of Pittsburgh

Virginia Tech

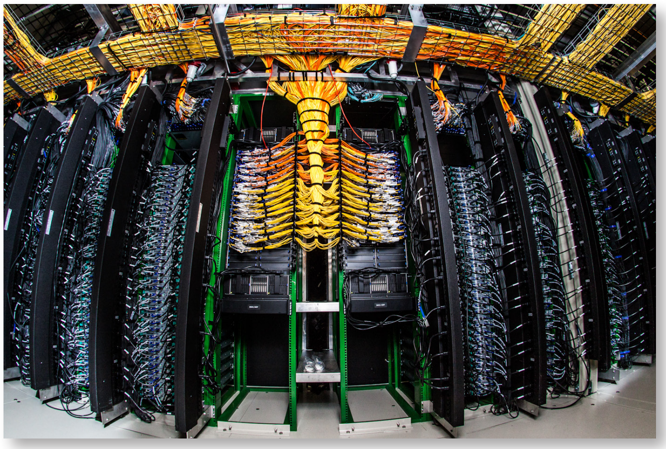
West Virginia University

URS Corporation

PARTNERS

SGI

NETL Carnegie Mellon PENNSTATE University of Pittsburgh URS VirginiaTech WestVirginiaUniversity



This image shows two of three Mellanox Infiniband 648-port switches, which are arranged in a Fat-Tree topology allowing for 40Gb/s non-blocking bandwidth between 1,512 computational nodes.

Visualization Centers: Improving Collaborative Efforts

The SBEUC facilities support effective collaboration among researchers and will improve interaction across NETL and its partnering NETL-Regional University Alliance (RUA) sites. In addition to secure desktop access for users, visualization centers—dedicated space for collaboration and simulation work— are installed at each of the three NETL sites: Morgantown, Pittsburgh, and Albany.

Additionally, a collaboration workstation is installed at each RUA site that includes high quality displays allowing group interaction and a more detailed exploration of simulation results. Users can also connect from off-site locations to monitor simulation progress outside of work and can share their simulation results with other SBEUC users.

Impacts and Benefits: Datacenter Efficiency

Recognized by Top 500 as one of the top 100 supercomputers in the world—currently ranked 55— the HPCEE is the most energy efficient for its size, using only 5.7 percent of its power for cooling versus 50 percent usage for traditional data centers. All of the computational, visualization, network hardware, and primary storage servers are installed in a high-efficiency modular datacenter. This approach leverages new free-air cooling technology and permits full operation of the computation systems with minimal cooling costs. This free-air cooling method operates by circulating filtered outside air through the datacenter and supplementing it with evaporative cooling, allowing the HPCEE to operate as one of the most efficient datacenters in the world.

An external shot of the modular datacenter shows the filters for the free-cooling air technology. Using this technology the HPCEE is able to operate with a Power Utilization Effectiveness (PUE) of 1.06—for every kilowatt of power used for computation only 60 additional watts are required for cooling.

NETL-RUA Regional University Alliance

the ENERGY lab

R&D FACTS

Geological & Environmental Sciences

NETL's Energy Data Exchange (EDX) – A Web-Based Tool to Coordinate Energy Research

Data Exchange for Energy Solutions

EDX™ Energy Data eXchange

Background and Benefits

The Energy Data Exchange (**EDX**; edx.netl.doe.gov) is an online coordination and collaboration platform developed by NETL's intramural research program to support subsurface energy research. Efficient and timely research has always been driven by access to existing information, the ability to quickly share and coordinate data with collaborators, and the ability to disseminate the results of work products as they develop. EDX supports these needs, offering timely access and coordination to data for researchers that require information associated with subsurface energy sources. In addition, EDX is utilized as a platform for rapidly disseminating NETL's research products.

EDX builds on NETL's experience in online tools such as the Knowledge Management Database (KMD) and NATCARB. KMD is a platform for disseminating results from DOE's oil and gas programs, including past technical reports and data. NATCARB is a platform for coordinating information on both CO_2 sources and potential CO_2 storage reservoirs, growing out of the efforts of the Regional Carbon Sequestration Partnership program. EDX extends these platforms in two ways:

- EDX incorporates a broad set of subsurface information common to CO_2 storage and other subsurface energy needs (e.g. shale gas, tight oil, deepwater and ultra-deepwater, and unconventional fossil resources). This set of information includes reservoir data, fluids properties, wellbore data, fault/fracture data, and groundwater data. Although some of the information resides in EDX as data derived from NETL research, much of the information exists online distributed in external databases. In these cases, EDX serves as a clearinghouse, allowing researchers to locate data rapidly by serving as a portal to these other datasets. Through this coordinated approach, EDX addresses one of the key lessons learned during DOE's work on the Deepwater Horizon oil spill--namely that locating and accessing data across a range of sources is challenging and often inefficient.

- EDX serves as a platform for disseminating research data both within projects, across projects, and externally. In this role, EDX facilitates coordination of both restricted-access and open-access research data and through the use of online visualization tools. EDX also facilitates seamless integration with researchers at collaborating institutions. Importantly, EDX can serve as an external platform, allowing the research team to "publish" data and reports easily from the secure internal collaboration platform to the open-access external technology transfer platform when appropriate.

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Ultimately, EDX seeks to ensure improved access to data and resources from a range of sources, offering a venue for the "publication" and dissemination of new datasets as well as historical, often inaccessible, assets ensuring their use for future, yet-to-be envisioned purposes.

Primary users of EDX are researchers actively engaged in work relevant to subsurface energy systems. However, the open-access resources within EDX can also be made available to the public, policy makers, commercial, and non-government organizations. EDX provides this access while helping to accelerate further research on pressing energy-related issues associated with oil, natural gas, the environment, and carbon management.

Functionality:

Core elements of EDX functionality are:

- An online platform for rapid and efficient access to priority datasets,
- Ability for researchers to share and "publish" online their data-driven products,
- A secure environment for multi-organizational research teams (including member researchers from DOE National Laboratories and other organizations) to share, build, and collaborate in a common workspace (available spring 2013), and
- Online tool to disseminate data, information, and results from DOE's Fossil Energy intramural research portfolios (e.g., the DOE EPACt Complementary Program, CO_2 Storage Program, National Risk Assessment Partnership (NRAP), National Methane Hydrates Program, etc.).

Datasets physically housed within EDX are provided by users either as links to external websites or when appropriate as standalone files such as Microsoft® Excel, .jpg, .zip, etc. Datasets can be "published" in their original and complete form in EDX and accompanied by associated reports, dissertations, or appropriate metadata. EDX also recognizes that there are significant established online resources and offers the ability to store links to external online data, thus improving coordination with existing resources to EDX users.

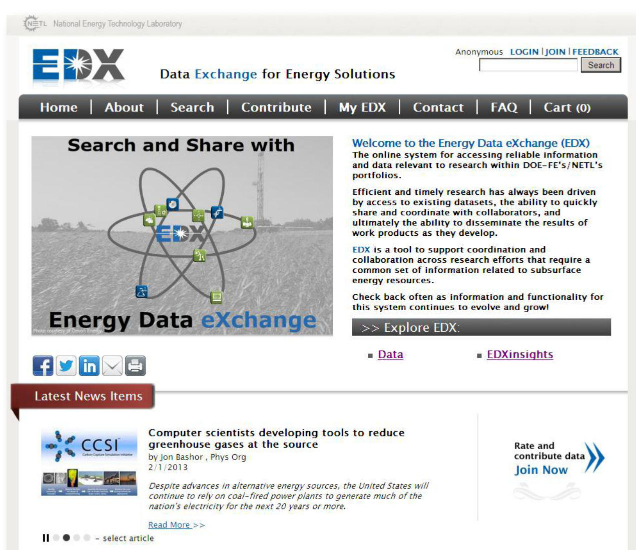
Contributing to EDX is quick, easy, and streamlined. The process begins by completing the online submission form where users can describe attributes, characteristics, and keywords of the submission. This information serves as the building blocks of EDX and is utilized to compile search results. Providing thorough and accurate information about the submission will enhance its visibility.

EDX Version 2:

Version 1 of EDX was released in July of 2012. Additional functionality and capabilities will be embodied in EDX Version 2, scheduled for release in the spring of 2013. EDX Version 2 will provide advanced coordination, collaboration, and data visualization functionality. The following features will be included in this deployment:

- EDX will support a variety of *Group Functionalities*, ranging from informal collaboration among a subset of colleagues that can be quickly created, to more formal and secure groups that will evaluate and verify the credentials of those requesting to join and participate. This functionality will augment the ability to restrict data to certain groups.
- The *Data Visualization Tool* will display files within EDX and assist in determining if the user would like to download those files.
- The *Collaborative Workspace* will be an environment where researchers can quickly and efficiently share data, ideas, and research techniques in a secure and dedicated work space.
- The *Rapid Response Tool* will be utilized in the event of a natural disaster, man-made catastrophe, or any other energy related event where news and data must be quickly coordinated and exchanged.

EDX will continue to evolve after deployment of Version 2 so check back often as information grows and functionality for this system improves. Registered users interested in options for specialty datasets and customized solutions can contact EDX Support at EDXsupport@netl.doe.gov.



Visit us at **www.edx.netl.doe.gov**

PROVIDING SOLUTIONS TO NATIONAL ENERGY CHALLENGES

NETL'S MATERIALS SCIENCE & ENGINEERING

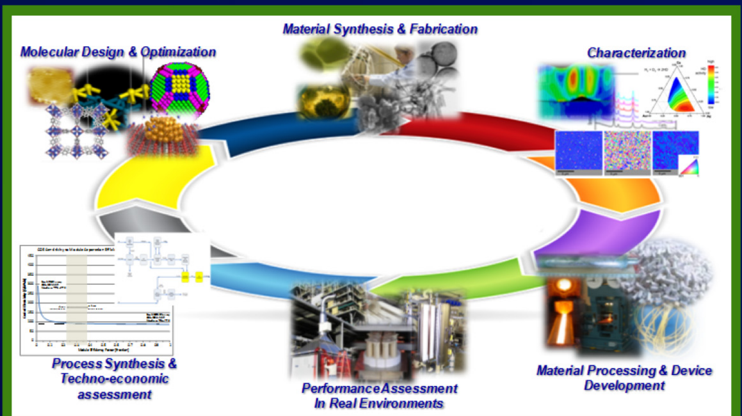
100 Years of Leadership and Innovation

For the last 100 years, the National Energy Technology Laboratory (NETL) has been on a quest to provide relevant materials solutions. At NETL, materials science inspires our researchers to embrace new perspectives and consider the impossible as they strive to answer industry's challenges. As an integral part of an internationally recognized, government-owned research facility, NETL's Materials Science & Engineering Focus Area (MSEFA) provides solutions to materials challenges facing the nation. The MSEFA is able to accomplish this mission through a combination of world-class facilities and a talented, multi-disciplinary staff.

Research Focused on Solutions

NETL's capabilities can be used to solve industry's most challenging materials requirements.The breadth of facilities and intellectual capital within the NETL enables the provision of solutions across the research and development continuum. Through existing competencies, NETL can assemble the right team using the right technology to arrive at the right solution in a timely and cost effective manner.

ACCELERATING DISCOVERY, DEVELOPMENT & DEPLOYMENT



MSEFA'S WORLD-CLASS CAPABILITIES

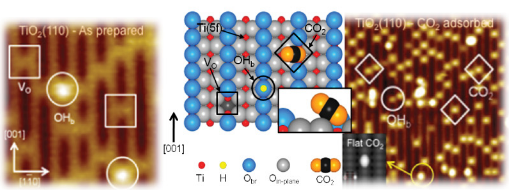
Materials	Approaches	Technologies
• Metal alloys & composites • Electro-ceramics • Polymers & composites • Molten salts • Nanomaterials • Refractory ceramics	• Design & optimization • Material synthesis • Characterization • Performance assessment • Processing & prototype • System integration & engineering and economic assessment	• Alloy manufacturing • Advanced combustion • Gas separations • Turbines • Reaction engineering • Solid oxide fuel cells • Refractory-based liners • Sensors • Batteries • Medical alloys

MSEFA has a long history of discovery, development, and deployment of affordable, high-performance materials and processes that overcome industrial challenges, including:

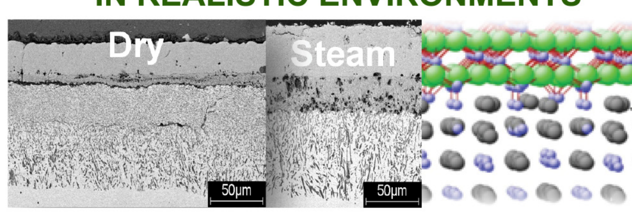
- Analyzing and developing corrosion-, erosion-, and wear-resistant materials able to withstand extreme environments.
- Computer modeling and simulation to accelerate product development and commercialization and to reduce verification and experimentation steps.
- Improving manufacturing by process improvement.
- Using advanced material capabilities to formulate, melt, cast, forge, and heat-treat materials on a prototype/industrial scale.

NETL's world-class research has been recognized by the scientific community, receiving fourteen R&D 100 awards over the past 5 years.

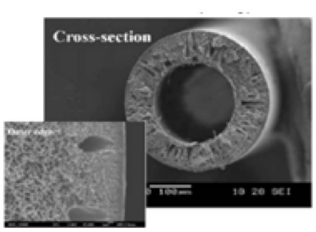
ADSORPTION PHENOMENON



EVALUATION OF MATERIALS IN REALISTIC ENVIRONMENTS

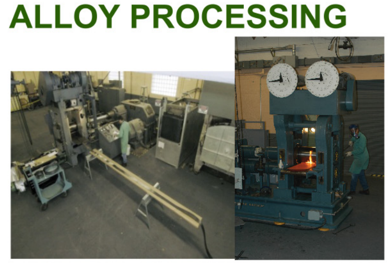


MATERIALS INTO DEVICES

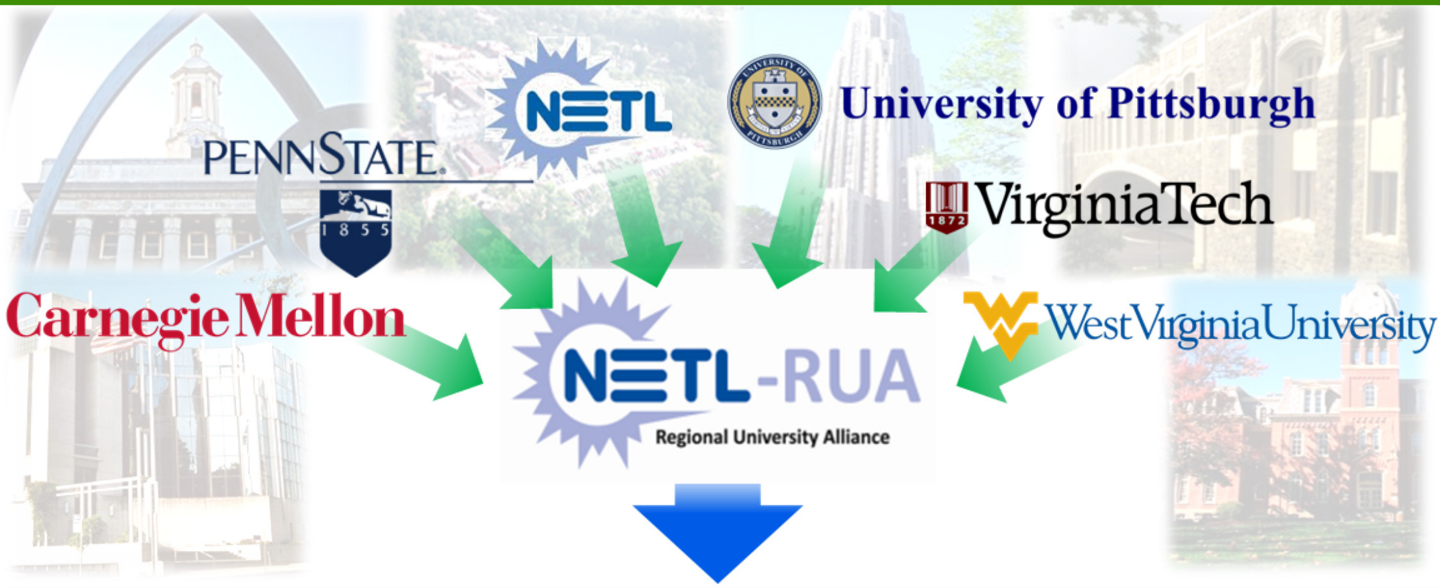


FIELD TRIALS

ALLOY PROCESSING



COLLABORATIVE R&D FOR TECHNOLOGY ADVANCEMENT



Shared Resources + Shared Intellect = Targeted Innovation

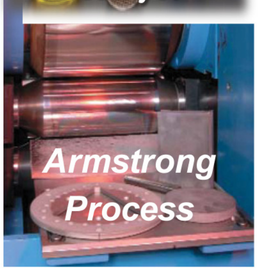
Create and enable **dynamic** teams to do **targeted** research that effectively provides solutions to the Nation's most challenging problems

Computational & Basic Sciences - Energy Systems Dynamics - Geological & Environmental Systems - Materials Science & Engineering

Technology Spotlight

In collaboration with Boston Scientific Corporation, NETL developed a novel platinum-chromium alloy for coronary stent applications. The revolutionary alloy allows for detection on x-ray devices while providing unprecedented flexibility and corrosion resistance. The technology has become the leading stent platform in the world accounting for more than $4 billion in sales since its introduction in 2010.

In collaboration with industry and academic partners, NETL validated and advanced its novel high-temperature, chemically stable catalyst for converting heavy hydrocarbons into hydrogen-rich synthesis gas for use in solid oxide fuel cells. This technology was licensed to start-up company Pyrochem Catalyst Corporation and is under development for commercial applications.



NETL and International Titanium Powder, LLC developed a process to produce titanium alloy powders in a continuous manner. The Armstrong Process significantly reduces temperature and pressure requirements as compared to conventional batch processing, significantly lowering production costs.

NETL welcomes the opportunity to build mutually beneficial partnerships with industry, academia, and other national entities to address material-related challenges.

WORKING WITH NETL AND ITS PARTNERS

About NETL

The National Energy Technology Laboratory, part of the U.S. Department of Energy's national laboratory system, is owned and operated by the Department of Energy (DOE). NETL supports DOE's mission to advance the national, economic, and energy security of the United States.

In addition to research conducted onsite, NETL's project portfolio includes R&D conducted through partnerships, Cooperative Research and Development Agreements, financial assistance, and contractual arrangements with universities and the private sector. Together these efforts focus a wealth of scientific and engineering talent on creating commercially viable solutions to national energy and environmental problems.

NETL has research facilities in **Albany, OR, Morgantown, WV, and Pittsburgh, PA.**

Partnership Arrangements

NETL has several different types of agreements for industrial collaborations. These include Cooperative Research and Development Agreements, Contributed Funds Agreements, and Nondisclosure Agreements. These instruments enable industrial partners to negotiate an agreement suitable for their needs including Go/No-Go decision points to ensure progress aligns with expectations. Once a technology is developed, it could be available for licensing.

More information about working with NETL's Material Science and Engineering Focus Area can be found at: **www.netl.doe.gov/onsite_research/materials-science.html**

Or you can contact us directly at: **materials.solutions@netl.doe.gov**