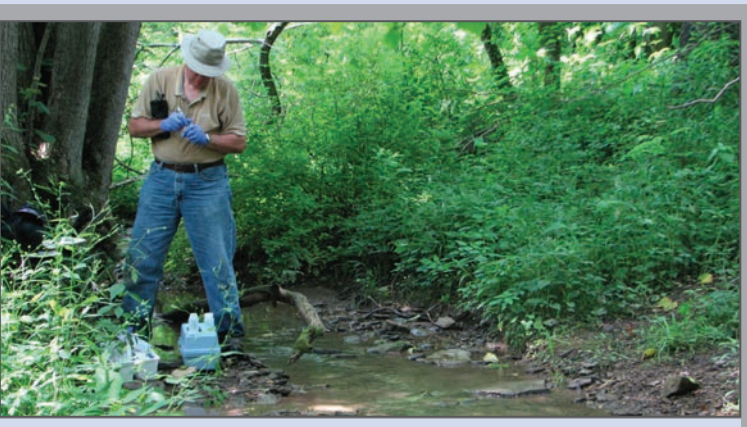
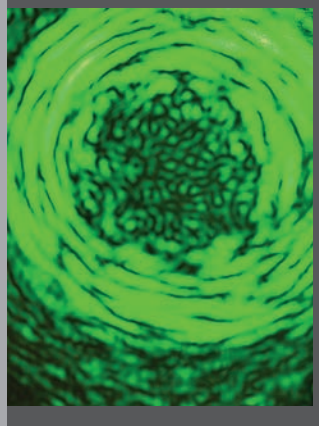
National Energy Technology Laboratory
Office of Research and Development

NETL-RUA Annual Review FY2012





DOE/NETL-2012/1579

U.S. DEPARTMENT OF ENERGY

NETL

Disclaimer

This document was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

NATIONAL ENERGY TECHNOLOGY LABORATORY REGIONAL UNIVERSITY ALLIANCE (NETL-RUA)

Annual Review FY2012

DOE/NETL-2012/1579

FINAL REPORT

June 2013

NETL-RUA Contact: Julianne Klara

National Energy Technology Laboratory

www.netl.doe.gov

Acknowledgments

The efforts described in this report were made possible through the funding and guidance provided by the NETL Strategic Center for Coal and Strategic Center for Natural Gas and Oil. The guidance and support of NETL Office of Research and Development (ORD) senior management and the NETL-RUA Executive Committee (EC) were crucial to the success of these research efforts.

The contents of this report reflect the hard work and dedication of a multitude of researchers from NETL, its five university alliance, and its site support contractor, URS, under U.S. Department of Energy (DOE) NETL contract No. DE-FE0004000. Support provided under DOE Contract No. DE-FE0004003 for the preparation of this report is gratefully acknowledged.

Special thanks to the following individuals who supported the preparation of this review: Nancy Andres[1], David Anna[1], George Guthrie[1], Bryan Morreale[1], George Richards[1], Jessica Sosenko[1], Madhava Syamlal[1], Richard Bajura[2], Andrew Gellman[2], Brian Gleeson[2], Dan Haworth[2], Roe-Hoan Yoon[2], Gabe Barki[3], Amanda Heaton[3], Tom Marshall[3], John Oelfke[3], Kelli Snedegar[3], Andrea Ware[3], Terry Summers[4], Paul Deffenbaugh[5], Lee Carnahan[5], Jane Engel[5], Jennifer Funk[5], Christy Pecyna[5], and Darcy Sucevich[5].

[1]NETL, [2]NETL-RUA Consortium Area Leads (CALs), [3]KeyLogic Systems Inc., [4]Smart Data Solutions, LLC, and [5]URS Corporation

Table of Contents

List of Abbreviations 6

Letters

Message from NETL's Director. 8

Message from NETL's Research and Development Director 8

Messages from NETL-RUA University Presidents 9

A Word from NETL-RUA's Manager 10

The Year in Review 11

Performing Innovative Research 15

Increasing Economic Impact 31

Accelerating Innovative Solutions 39

Preparing Tomorrow's Energy Leaders 43

Operations 50

NETL-RUA Executive Committee 50

NETL-RUA at a Glance 51

Outreach and Impact 52

What to Expect in 2013 63

Appendix A: FY2012 NETL-RUA Research Teams and Personnel 65

Appendix B: FY2012 NETL-RUA Peer-Reviewed Publications. 81

NETL-RUA Contacts. 92

Abbreviations

a-Si	amorphous silicon
ADA-ES	ADA Environmental Solutions, Inc.
AIChE	American Institute of Chemical Engineers
ALAMO	Automated Learning of Algebraic Models for Optimization
APU	auxiliary power unit
A-USC	advanced ultrasupercritical
AVESTAR™	Advanced Virtual Energy Simulation Training and Research
BIAS	Basic Immobilized Amine Sorbent
BSCI	Boston Scientific Corporation Inc.
C3M	Carbonaceous Chemistry for Computational Modeling
CAL	Consortium Area Lead (University)
CCR	Council for Chemical Research
CCSI	Carbon Capture Simulation Initiative
CFD	computational fluid dynamics
CLC	chemical looping combustion
CMRA	Critical Materials Research Alliance
CMU	Carnegie Mellon University
CO_2	carbon dioxide
CRADA	Cooperative Research And Development Agreement
DD	Division Director
DOE	Department of Energy
E&I	Energy and Innovation
EC	Executive Committee
EDX	energy data exchange
EMS	Earth and Mineral Sciences
EPA	Environmental Protection Agency
EPACT	Energy Policy Act
ESR	Electro Slag Remelting
FE	Fossil Energy
FEB	Federal Executive Board
FLC	Federal Laboratory Consortium
FOA	Funding Opportunity Announcement
FWP	Field Work Proposals
FY	fiscal year
GE	General Electric
GHG	greenhouse gas
GTC	Grid Technologies Collaborative
HENAAC	Hispanic Engineer National Achievement Awards Corporation
IAM	integrated assessment model

ICMI	Industrial Carbon Management Initiative
IGCC	integrated gasification combined cycle
IPT	Innovative Process Technologies
LIBS	laser-induced breakdown spectroscopy
Li-ion	lithium ion
MFIX	Multiphase Flow with Interphase eXchanges
MOSS	Members Only SharePoint Site
NAE	National Academy of Engineering
NAS	National Academy of Sciences
NATCARB	National Carbon Sequestration Database and Geographic Information System
NETL	National Energy Technology Laboratory
NETL-RUA	National Energy Technology Laboratory-Regional University Alliance
Ni	nickel
NRAP	National Risk Assessment Partnership
OASIS	omicron analysis and surface imaging system
ORD	Office of Research and Development
PCC	Pyrochem Catalyst Corporation
PECASE	Presidential Early Career Award for Scientist and Engineers
Penn State	Pennsylvania State University
PI	Principal Investigator
Pitt	University of Pittsburgh
R&D	Research and Development
SBEUC	Simulation-based Engineering User Center
SECA	Solid State Energy Conversion Alliance
SERA	Shale Energy Resources Alliance
SGA	Strategic Growth Area
Si	Silicon
SOFC	solid oxide fuel cell
STEM	science, technology, engineering and math
SwRI	Southwest Research Institute
T&D	transmission and distribution
UDW	Ultra-Deepwater
UNIGE	University of Genoa
USDA	United States Department of Agriculture
Virginia Tech	Virginia Polytechnic Institute and State University
WVU	West Virginia University

"We brought together five major universities, a very multifaceted government organization, and a major company to channel efforts and focus on a singular goal of building a regional powerhouse that could do fantastic, cutting-edge research."

—Anthony Cugini, Director, National Energy Technology Laboratory

"NETL-RUA delivers a powerful combination of capability and expertise to serve as an engine for energy innovation for the region, the nation, and the world."

—Cynthia Powell, Director, Office of Research and Development, National Energy Technology Laboratory

Messages from NETL-RUA University Presidents

Jared Cohon

President, Carnegie Mellon University

"NETL is the anchor of a regional research network that is advancing breakthroughs to transform America's energy future. Working with NETL, the RUA partners are committed to speeding technologies from the lab to commercialization and deployment and to establish a new model for university/federal laboratory collaboration."

Rodney Erickson

President, Pennsylvania State University

"Many of our faculty members have already had some collaborative research and scientific exchange. This type of intellectual exchange fosters understanding and can lead to discoveries that will benefit our institutions, our nation, and the world."

Mark Nordenberg

Chancellor, University of Pittsburgh

"The University of Pittsburgh is proud to be partnering with four other outstanding universities on the Regional University Alliance. Our five universities have a combined total research portfolio in excess of $2 billion and have highly complementary strengths in energy research. Our alliance with NETL creates a powerful partnership at a time when energy research is a top national priority – in terms of economic growth, national security, and environmental stewardship."

Charles Steger

President, Virginia Polytechnic Institute and State University

"With 200 researchers focused on environmentally friendly and sustainable energy, Virginia Tech is committed to working with its NETL-RUA partners to develop existing domestic energy resources and new materials. Our efforts will help propel the United States into the new, clean energy economy, energize our country's high-technology manufacturing industry, and preserve the environment for generations to come."

James Clements

President, West Virginia University

"As the flagship, land grant university of one of the nation's leading energy producing states, West Virginia University is committed to providing the ideas, talent, and leadership needed to address global energy concerns through collaboration in education, discovery, and innovation. We know that the NETL-RUA partnership, combining the talent of five of our nation's leading research universities with that of the National Energy Technology Laboratory, will help enable the U.S. to lead the world in the development of innovative solutions to address the growing global demand for energy."

A Word from NETL-RUA's Manager

Three key goals of NETL-RUA are to develop transformative science and technology solutions that will lead to a sustainable energy future, use research as a springboard to develop the energy leaders and entrepreneurs of tomorrow, and serve as a source of regional economic development and nationwide job creation. In its second full year of operation, NETL-RUA has made significant strides in all three of these areas.

NETL's mission-critical research, performed by federal researchers working with university and industry researchers of NETL-RUA, has resulted in discoveries that will lead to efficient reduction of the carbon footprint of fossil energy systems, economical utilization of produced carbon dioxide, and safe production of domestic fossil resources that move us toward energy independence. Through joint NETL-RUA investment to seed several key initiatives, known as "Strategic Growth Areas," NETL-RUA teams are pursuing opportunities that capitalize on the unique nexus of capabilities and expertise borne from NETL-RUA fossil energy research to address a broader array of energy-related issues. These areas include critical materials, grid technology, and shale gas, all of which are supported by the cross-cutting technologies of advanced materials and computational science. In all of these efforts, NETL-RUA researchers have worked together to create stronger teams and offer more robust research plans in pursuit of expanding research and development efforts. In the two years since its inception, NETL-RUA has seen a measurable increase in these collaborative efforts, resulting in increased opportunities for new research that will have a positive effect on economic growth, environmental stewardship, and energy security.

This year, over 40 students obtained advanced degrees as part of NETL-RUA confirming the program's commitment to engage students in cutting-edge energy research. Through its ability to provide real world experience and offer hands-on education for engineers and scientists, its partnerships with manufacturers and industry, and its focus on market-based applications, NETL-RUA continues to serve as a key source of regional economic development and nationwide job creation. The prestigious awards and other recognition achieved by NETL-RUA researchers described in this report indicate that the impact and value of NETL-RUA research has been acknowledged by peers in the technical community.

Through a targeted strategy developed for the coming year, NETL-RUA will build on the success achieved in this second year of fossil energy research, strategic growth, and educational initiatives to have an even greater positive impact on the future of energy.

Respectfully,

Julianne M. Klara
NETL-RUA Manager
Office of Research and Development
National Energy Technology Laboratory

The Year in Review

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-RUA (or Alliance), a government-university-industry energy research partnership established in January 2010.

This alliance combines the facilities, expertise, and resources of NETL with those of five world-renowned research universities—Carnegie Mellon University (CMU), the Pennsylvania State University (Penn State), the University of Pittsburgh (Pitt), Virginia Polytechnic Institute and State University (Virginia Tech), and West Virginia University (WVU)—as well as industry partner URS Corporation, one of the nation's largest and most comprehensive engineering services firms.

Top scientists and engineers from NETL, URS, and five regional university partners are working to develop solutions that will enable the responsible, sustainable utilization of our nation's fossil energy (FE) resources, and create the innovative technology platforms that will be needed to transition to a sustainable energy future.

The Alliance made significant strides toward meeting all four key strategic goals during the fiscal year (FY) 2012 period from September 1, 2011 through October 31, 2012.

NETL-RUA Key Goals:

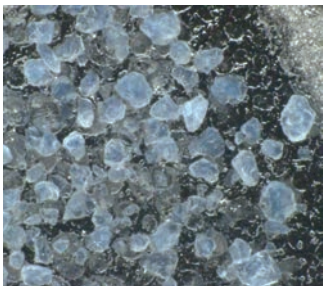
1. Perform innovative, collaborative research to meet U.S. demand for energy, power, fuels, and chemicals from fossil fuels and allow for a smooth transition to a sustainable energy future
2. Increase the economic impact of the research and development (R&D) portfolio through new opportunities and markets
3. Accelerate commercialization of advanced technologies through cooperative programs
4. Prepare tomorrow's energy leaders

Innovative Research

NETL-RUA researchers have collaborated to achieve some key innovations in FY12. These revolutionary technologies have the potential to dramatically increase the performance of processes to reduce the carbon footprint of FE systems and enable super-efficient advanced power production systems.

Key technology developments include:

- The **Basic Immobilized Amine Sorbent (BIAS)** process was recognized by *R&D Magazine* as among the 100 most technologically significant products introduced into the commercial marketplace within the past year. The BIAS sorbent technology is capable of capturing carbon dioxide (CO_2) from flue gas at a cost lower than that of conventional systems and shows promise for other applications such as natural gas purification and conversion of landfill emissions to fuel.



Basic Immobilized Amine Sorbent

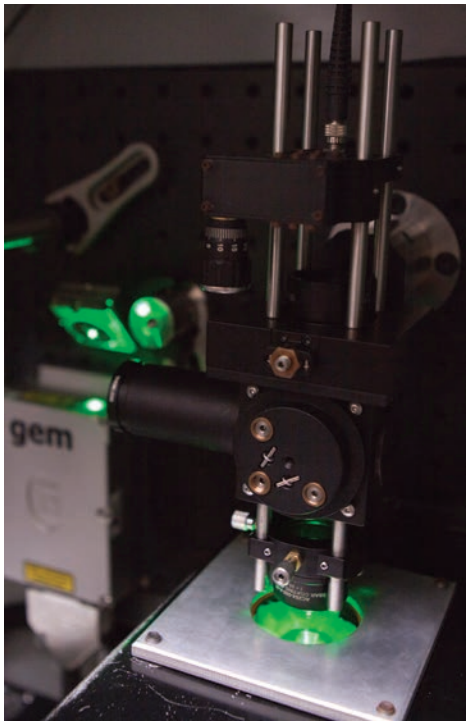
- Developed by a partnership of National Laboratories (Los Alamos National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, NETL, and Pacific Northwest National Laboratory, and led by NETL ORD, the **Carbon Capture Simulation Initiative (CCSI) Toolset** consists of modeling and simulation software that will help reduce the cost of and time to complete various stages of carbon capture technology development (from the discovery of new materials to the deployment of new technologies) with the expectation of reducing development time by about 25 percent.

- Researchers developed the "most efficient" approach ever reported to convert CO_2 to useful chemicals. This **catalyst concept for CO_2 utilization**, which uses the lowest possible energy input on a thermodynamic basis, may provide an efficient and cost-effective pathway for converting unwanted CO_2 emissions from FE systems to chemicals and other value-added products.

- A **homogenization heat treatment for cast alloys** was developed that provides a computationally-based procedure for producing thick-section metal alloy castings. This process helps produce uniform and consistent high-temperature mechanical properties resulting in creep performance rivaling that of forged product of the same alloys. This is an enabling technology for high-efficiency advanced power systems.

- **Cathode technology for solid oxide fuel cells (SOFCs)** that can increase SOFC performance by 40 percent, while decreasing costs by a similar percentage, has been demonstrated by researchers in lab tests to have exhibited stable cathode performance for more than 1500 hours. This technology is being transferred to the private sector for pilot-scale testing.

- A **real-time sensor for gas composition** has been developed that, unlike existing approaches that require several minutes to analyze a gas blend, can make measurements in less than one second for natural gas and most other gas mixes of interest to advanced power systems. This sensor technology will be used to measure coal syngas composition at the Wilsonville National Carbon Capture Center, and may be applied to characterize gas composition in chemical conversion facilities.



Raman gas composition sensor system makes real-time measurements in less than one second.

- **Advanced Virtual Energy Simulation Training and Research (AVESTAR)**, a high-fidelity, real-time dynamic simulator with a full-scope operator training system and a first-of-a-kind 3-D virtual immersive training system, provides hands-on, simulator-based, industry workforce training and engineering education on the operation and control of clean energy systems. It also enables the conduct of collaborative R&D on dynamic process modeling, advanced process control, optimal sensor placement, 3-D virtual plant technology, smart manufacturing, operational excellence, and modern grid applications.

Using the Virtual Plant at AVESTAR, plant conditions can be modeled in real time and visualized in 3-D for education and research.

Economic Impact

To increase the economic impact of NETL-RUA's research portfolio, its members have leveraged core capabilities and expertise to successfully garner over $2 million in joint Alliance proposals, expanded university research efforts by over $30 million in grant and contract awards, and submitted an NETL-RUA proposal worth $120 million to DOE's Energy Innovation Hub—Critical Materials funding opportunity announcement (FOA), the award of which was still pending at the end of FY12.

Commercialization

Accelerating commercialization of advanced technologies has been accomplished by identifying potential intellectual assets and working to convert them into new products, processes, and jobs. Twelve patents were issued during FY12, including those for a laser-based analytical technique to perform real-time chemical element measurements to monitor CO_2 leakage, seal integrity, and Marcellus shale gas and water; a novel, low-cost approach for assembling a new anode for lithium ion batteries that results in a four- to five-fold increase in storage capacity; and a deactivation-resistant catalyst that disrupts the formation of carbon, a key contributor to deactivation of fuel reforming catalysts.

Tomorrow's Leaders

NETL-RUA continued its efforts to establish collaborative energy education programs using its research as a springboard by engaging 115 graduate and undergraduate students in NETL-RUA projects. Forty-one student researchers obtained advanced degrees in FY12 while working on NETL-RUA funded research. Additionally, NETL-RUA projects have been incorporated into some university business plan coursework as case-studies. One such project had significant success in national and international business plan competitions and has led to the formation of a start-up company based on NETL's patented R&D 100 award-winning cerium oxide coating for metallic alloys.

DANGER

Performing Innovative Research

Develop advanced energy systems based on sound science and consistent with the sustainable use of energy and environmental resources to meet present and future challenges in the production of energy, power, fuels, and chemicals.

FE Research

Our ability to meet the current and future energy needs of a global society will depend on the sustainable use of energy and environmental resources. Innovative solutions are being developed to transform today's FE technology into highly efficient, affordable, and clean advanced energy systems of the future.

NETL-RUA research is focused on addressing the grand challenges of reducing the environmental footprint of FE utilization for power, fuels, and chemicals and ensuring energy security by developing safe and affordable technologies for producing our nation's domestic resources.

NETL-RUA draws on resources from all of its partners to create research teams with experience, talent, renowned capabilities, and world-class facilities to discover, develop, and deploy next generation technologies.

The research being conducted by NETL-RUA is managed through thirteen collaborative research teams, comprising researchers from NETL, the Alliance universities, and site support contractor URS. This research also encompasses R&D partnerships with industry and other national laboratories to ensure that technologies under development effectively meet the emerging scientific and technological needs of the market.

The following is a summary of the major FY12 research accomplishments in each key FE research area.

Objectives:

1. Create and enable the right research teams to conduct the right research that effectively meets emerging national needs for science and technology.
2. Build R&D partnerships with the capability and expertise to be a force in the discovery, development, and deployment of next generation technologies.
3. Discover and develop the technologies that will launch the next energy economy.

A benefit of the 3D Virtual Plant at AVESTAR is the added dimension of plant realism and familiarization.

Coal Research

The primary focus of NETL-RUA coal R&D is to produce technologies that will increase fossil system efficiency and reduce emissions. Improved system performance preserves domestic natural resources while reducing the cost of controlling pollution and capturing and sequestering greenhouse gases (GHGs), all of which lead to greater energy and economic security.

Advanced Combustion

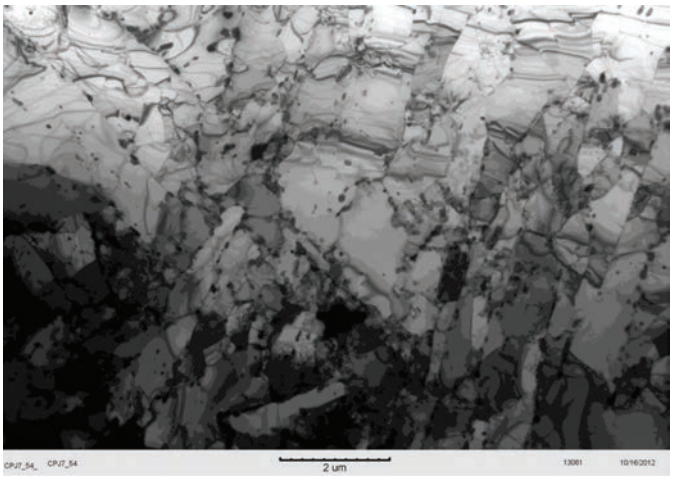
To improve the efficiency of conventional power generation, and thus reduce fuel consumption and lower GHG emissions, the NETL-RUA Advanced Combustion research team is conducting laboratory- through pilot-scale tests of advanced combustion technologies and systems capable of improving CO_2 capture performance with a minimal increase in the cost of electricity.

Oxy-combustion technology, in which oxygen is used instead of air for combustion, results in flue gas with a much lower nitrogen content, making it easier and more efficient to capture, utilize, and sequester produced CO_2. Further, the higher operating temperatures of the oxy-combustion system allow for a more efficient steam cycle for power generation.

A key objective of advanced combustion research is to develop boiler alloys that can withstand higher pressures and temperatures than current commercial systems. NETL's advanced ultra-supercritical (A-USC) steam autoclave provides researchers with the unique capability to examine fundamental issues of steam-side corrosion as functions of temperature and pressure.

In late FY12, shakedown tests of NETL's A-USC steam autoclave achieved supercritical steam conditions with good pressure control and permitted researchers to study, for the first time, material response to steam oxidation at proposed boiler/steam turbine steam pressures for A-USC power plants. In fact, the unit achieves greater than 265 bar pressure, which surpasses the pressure capability of other national laboratory autoclave systems in the United States and United Kingdom.

Research is also focused on designing alloys and developing manufacturing processes that can be practically and economically utilized to produce full-scale components for deployment. Research on nickel (Ni) superalloys has focused on alloy design, manufacturing process control, and heat treatment to produce homogenized high-quality Ni-based castings and steel forgings.



Transmission electron micrograph of martensitic steel CPJ-7

The NETL-RUA Advanced Combustion research team designed and manufactured ferritic-martensitic steels (designated CPJ-7-14) at NETL during the past year. One such steel, CPJ-7, has shown significant improvement in creep strength compared to existing state-of-the-art commercial power plant steels. This new martensitic steel could replace Ni-based alloys in USC steam turbines at temperatures up to about 635 °C at a significantly reduced cost for equal performance. A provisional patent application has been filed for this ferritic-martensitic steel.

NETL-RUA collaborated with industry partners in FY12 to facilitate the development of large-scale Ni-based superalloy castings for power plant applications. A portion of the research centered on achieving homogenized structures using a computationally-based heat treatment schedule that resulted in optimal mechanical behavior for the cast components. Researchers from the NETL-RUA Advanced Combustion team worked in particular with General Electric Company (GE) and its casting vendors to develop thick section Ni superalloy casting technology.

NETL-developed, computationally-based homogenization procedures have also been used to heat treat up to 1000 pound castings of Haynes 282 and alloy 263 that had uniform microstructures with little to no segregation and consistent high-temperature mechanical properties. Use of the computationally-based homogenization schedule prior to final aging for strength resulted in creep performance rivaling that of the more expensive forged versions of these same alloys.

Turbine Thermal Management

Gas turbine technology is directly linked to our nation's economic and energy security. The NETL-RUA Turbine Thermal Management research team takes an integrated, systematic approach to advancing thermal protection of turbine hot sections such as first-stage vanes and blades and control of secondary flows.

Turbines have been the world's energy workhorses for generations. They are the heart of almost all of the world's electric generating systems.

Significant advances in turbine cooling effectiveness, as well as thermal barrier coating performance and durability, are needed for turbine operation at the high temperatures and pressures required by future high-efficiency, near-zero emission turbine power systems.

NETL-RUA research projects utilize the extensive expertise and readily available facilities at NETL and participating universities and are being undertaken by a highly collaborative and interactive materials and heat transfer team consisting of major land-based turbine original equipment manufacturers (Siemens Energy, Pratt & Whitney) and at industrial manufacturing sites (Mikro Systems Inc., Howmet International, PCC), small business partners (Coatings for Industry), industrial stakeholders (GE, Siemens, Solar, Pratt & Whitney, universities, Southwest Research Institute [SwRI], FTT, etc.), and other government agencies (NASA GRC, Ames Laboratory).

The overall NETL-RUA research approach includes explorative studies based on scaled models and prototype coupon tests conducted under realistic pressure and high-temperature turbine operating conditions. In conjunction with these efforts, a world-class NETL-RUA rotating turbine test facility is being designed and constructed at Penn State in collaboration with Pratt & Whitney that, when completed, will address leakage, secondary flow, and internal heat transfer in high speed rotating turbine airfoils.

Turbine materials development efforts in FY12 included evaluation of advanced material system architectures on airfoil metal substrates with extreme thermal barrier coated systems for operation at temperatures greater than 1400 °C.

Efforts to expand the materials portfolio also included development of integrated oxide dispersion strengthened systems for use with NETL-RUA's near surface embedded micro-channel concept for enhanced airfoil surface cooling, and leveraging ceramic matrix composite technologies for use at turbine inlet temperatures between 1500 and 1600 °C.

These concepts to further increase the cooling effectiveness of internal and film cooling designs are being converted to prototype, first-of-a-kind, cast test coupons for heat transfer performance evaluation in NETL's high temperature/pressurized aerothermal test facility.

Advanced Gasification

The outstanding environmental performance of gasification makes it an excellent technology for the clean production of electricity and other products such as fertilizer or feedstock chemicals used in the manufacture of plastics.

The NETL-RUA Advanced Gasification research team focuses on optimizing gasification systems to facilitate cost-effective gasification of both high- and low-rank coals and alternative feedstocks such as petcoke and biomass, improving system components and materials, and developing models designed to increase system efficiency, reliability, and reduce manufacturing costs.

The team made significant progress in refractory improvements and low-rank coal optimization. The team developed software to predict slag properties and collected the first thermodynamic data for low-oxygen, partial vanadium compounds that can be used to predict properties of petcoke feedstock—data that is essential for predicting slag behavior and controlling the gasification process. This work, though in its early stages, was recognized by the American Ceramic Society as the most important phase diagram work of 2012.

NETL-RUA is also developing predictive models of coal particle gasification by analyzing actual carbon feedstock particle size fractions to predict their impact on gasification efficiency, the fluidity of mineral impurities, particle buildup on heat exchangers, and the physical state of various materials during the gasification process. This information provides insight into preparing materials for gasification and controlling/minimizing gasification material issues.

The NETL-RUA Advanced Gasification research team continues to be at the forefront of reactive multiphase flow simulation. A new version of Carbonaceous Chemistry for Computational Modeling (C3M), the world's largest virtual reaction kinetics laboratory for coal and other carbonaceous materials, was developed and delivered to industry in FY12.

The C3M helps bridge the gap between reliable chemistry and computational models of reacting, multiphase systems with the tools needed to build and understand complex chemistry models.

Further, a new version of the open-source simulation code Multiphase Flow with Interphase eXchanges (MFIX), which includes several advances in its underlying physics and geometric modeling capabilities, was launched. These modeling tools continue to impact reactive multiphase flow simulation directly through application of gasifier and carbon capture device modeling and indirectly through dissemination to industry through commercial simulation software and academic research applicable to FE systems. MFIX has over 3000 registered users, including 384 new registrations in 2012 (73 percent universities, 15 percent industry, and 12 percent others).

Optimizing coal-based processes depends on efficiently removing harmful emissions of mercury, arsenic, and selenium derived from coal utilization. This research team has been instrumental in developing patented materials for synthesis gas cleaning at elevated temperatures to meet new U.S. Environmental Protection Agency (EPA) mercury emissions requirements (which are considered to be the most difficult to meet). Patented materials for

warm-gas cleanup have been developed, licensed to Johnson Matthey, undergone successful industrial testing at Southern Company, and have received an R&D 100 award. A total of six patents have been awarded and two R&D 100 awards received in the area of warm-gas cleanup.

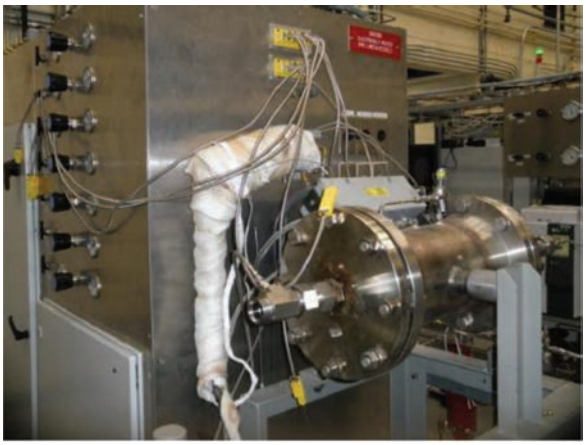
FY12 also saw the launch of NETL's AVESTAR™ Center, a high-fidelity, real-time dynamic simulator with operator training and first-of-a-kind 3-D virtual immersive training for an integrated gasification combined cycle (IGCC) power plant with CO_2 capture. This innovative virtual reality technology—when combined with AVESTAR's state-of-the-art, real-time, high-fidelity IGCC dynamic simulator—provides engineers, operators, researchers, and students with hands-on operations, control, and safety training in a highly realistic, integrated, IGCC plant and control room environment.

The NETL-RUA Advanced Gasification research team uses AVESTAR to conduct internationally-recognized collaborative R&D on dynamic process modeling, advanced process control, optimal sensor placement, 3-D virtual plant technology, smart manufacturing, operational excellence, and modern grid applications.

Fuels

Coal—America's most plentiful domestic FE resource—has the potential to produce abundant, economically attractive hydrogen, and other clean fuels to both increase energy security and reduce CO_2 emissions. Development and demonstration of syngas conversion technologies will facilitate the production of affordable fuels, intermediate chemicals, and power from coal-based feeds.

The NETL-RUA Fuels research team is focused on developing and assessing technologies such as catalysts and separation materials that can facilitate gas conversion reactions and be used in severe environments associated with syngas conversion for extended periods while retaining their beneficial properties. The overall objective is to significantly advance the development of low-cost membrane materials and architectures that have high hydrogen selectivity, provide appropriate hydrogen fluxes, and resist degradation by syngas-laden contaminants.



A high pressure (up to 1000 psi), high temperature (up to 900 °C) test reactor used by NETL-RUA researchers to develop and test materials in a syngas environment.

Hydrogen separation technologies are being tailored to conditions consistent with post-warm gas cleaning and integration into water-gas shift technologies. Recent studies have revealed the potential for significant uptake of the contaminants arsenic and selenium into the separation alloy upon exposure to even low levels of these species.

Systems studies have indicated that development of a more durable membrane that can function under real operating conditions may be more important than simply focusing on a hydrogen flux target. 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 is also focused on developing catalytic materials that can utilize typical fossil gas constituents as a replacement for petroleum feedstocks to create transportation fuels, chemicals, or other value-added products. For example, over 90 percent of the industrial chemicals benzene, toluene, and xylene are currently derived from petroleum naphtha. Successfully developing materials and processes to create these chemicals from C1 through C3 gas species can potentially replace a significant portion of petroleum feedstock. While incremental improvements in efficiency and selectivity have been made, success will depend on a combination of catalytic conversion and product removal, where shortcomings of equilibrium-limited reactions can be overcome.

Fuel Cells

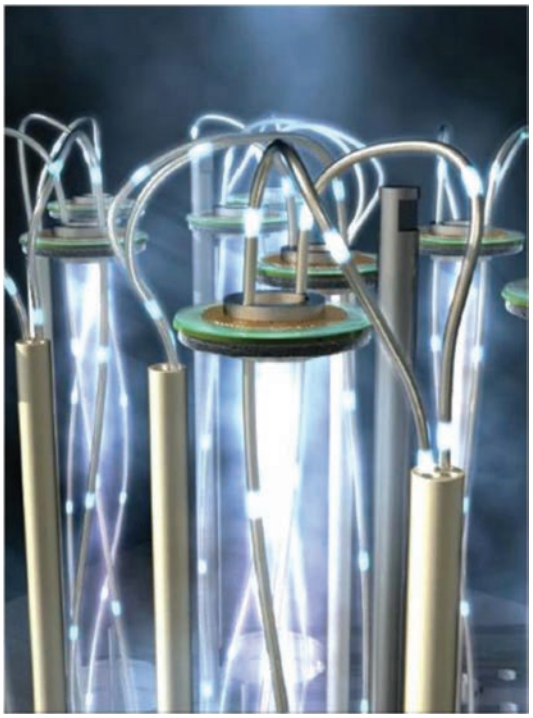
Fuel cells directly convert chemical energy to electrical energy using fuels such as coal and natural gas, bio-fuels, diesel, and hydrogen. Fuel cells are envisioned as supporting technical solutions to contemporary challenges in national security, the environment, fuel availability, and energy security. Fuel cells have the potential to enable high efficiency in central generation applications, present diverse opportunities for carbon capture, reduce criteria pollutant emissions, and conserve water.

NETL-RUA has diverse fuel cell testing and analytical capabilities that it is using to develop innovative new materials and evaluate the performance of fuel cells developed in DOE's FE Program. One major component is a multi-cell array test platform that has been used to examine fuel cell durability on coal synthesis gas. This unique experiment has allowed NETL-RUA researchers to characterize fuel cell lifetime subject to direct exposure to coal impurities, and thereby establish target synthesis gas cleaning levels.

The NETL-RUA Fuel Cell research team's objectives are to reduce stack costs and increase cell efficiency and stack longevity. Research is focused on investigating degradation processes of anode/electrolyte/cathode components as well as engineering electrode materials and microstructure.

The team's accomplishments include development of a cathode infiltration technology that can increase SOFC power performance by more than 40 percent. This power density increase corresponds to an equivalent cell stack cost reduction, and the materials impart enhanced stability in operational tests lasting more than 1,500 hours. This technology is currently being transferred to the private sector through industry collaboration focused on scaling it to commercially relevant scales (> 100 cm^2 active area).

The Fuel Cell research team also identified degradation modes associated with syngas fuel, air, and length of operation that diminish fuel cell stack lifetime and reduce reliability. Methods to mitigate two specific problematic modes were developed in collaboration with two industrial partners in DOE's Solid State Energy Conversion (SECA) program. NETL-RUA is now developing models to support commercial operation in a full-scale application, targeting a 200 percent increase in cell stack life with a resulting decrease in the cost of electricity.

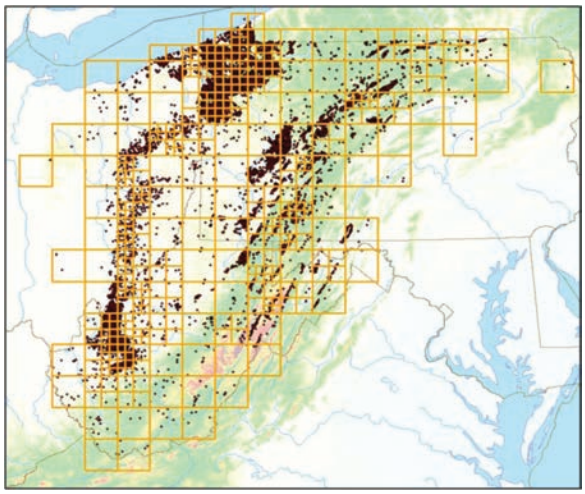


Shown above is a cutaway image of the NETL-RUA Fuel Cell research team's multi-cell array during operation. Each fuel cell converts chemical energy directly to electrical energy through a high-efficiency electrochemical reaction.

Carbon Storage

The NETL-RUA Carbon Storage research team is conducting research aimed at developing technologies that will significantly improve the safety and permanence of geologic CO_2 storage. Research includes developing estimation techniques for geologic storage capacity and permanence; technologies for monitoring, verifying, and accounting for CO_2, brine, and pressure plume migration into groundwater and air; and simulation and risk assessment tools for predicting processes affecting porosity and permeability. The research activities involve applied laboratory and pilot-scale experiments as well as numerical modeling.

Estimation techniques for geologic storage capacity were improved with the launch of the National Carbon Sequestration Database and Geographic Information System (NATCARB). This interactive online tool integrates information on North American CO_2 sources and potential storage reservoirs with ongoing research and demonstration projects in a publicly available, user-friendly mapping tool.



In order to more accurately evaluate CO_2 storage potential, a variable grid approach is applied to the Oriskany formation. This allows the availability of data to guide spatial analysis and interpolation methods when data density is not constant.

Additionally, the team developed a new geospatial analysis approach to characterize, interpret, and display subsurface geologic characteristics from well log entries to provide detailed inputs needed for assessing prospective CO_2 storage capacity. This new geospatial approach is tied to higher density of subsurface data for improved spatial resolution and characterization. The goal of this work is to assess capacity to ±30 percent to facilitate CO_2 storage.

The Carbon Storage research team has also developed a comprehensive suite of monitoring techniques for detecting CO_2 migration to the near-surface. The techniques focus on detection of tracers as well as potential changes in groundwater chemistry. These techniques allow operators to simultaneously confirm permanent storage of CO_2 and that groundwater is not being contaminated.

Results from NETL-RUA experiments on CO_2/brine/rock interactions under sequestration conditions indicate that CO_2-induced mineral dissolution and precipitation can result in significant changes to the permeability of the formation rock, which will have an impact on the potential rate of injection in the field. These results reinforce the importance of considering mineral reactivity in site characterization/evaluation.

Carbon Capture

Carbon capture and storage from fossil-based power generation is a critical component of a realistic strategy to prevent an increase in atmospheric CO_2 concentration, but capturing substantial amounts of CO_2 using current technology would result in a prohibitive increase in the cost of producing energy.

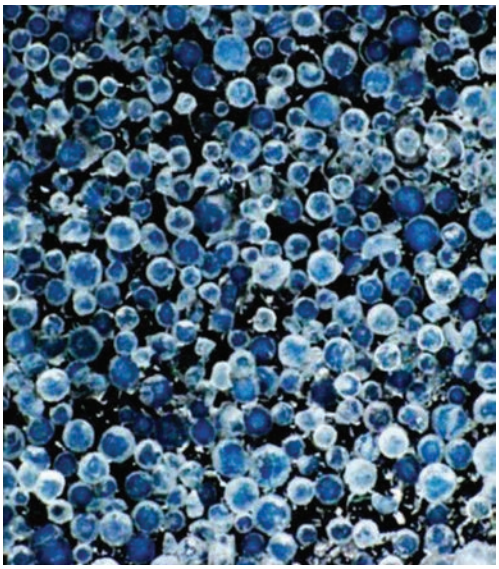
Ionic liquids created by NETL-RUA's Carbon Capture team have found application as CO_2 solvents, membrane transport phases, and electroplating media.

NETL-RUA is pursuing a multifaceted approach that 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.

NETL-RUA's capture program seeks to create technological solutions for carbon capture from pulverized coal power plants, IGCC plants, and oxy-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-combustion cycles require large amounts of oxygen, which is expensive to produce and adds considerable cost to the processes; therefore, NETL-RUA is also exploring new materials for selectively separating oxygen from air.

Current research is accelerating development of solvents, sorbents, and membranes by pursuing complimentary computational and experimental approaches.



Sorbent pellets of immobilized polyethylenimine on the support CARiACT Q10, a commercial silica gel support with a diameter of 100 to 350 um. Sorbent pellets were prepared in two 600-lb batches by Pressure Chemical Company.

A solid sorbent capable of capturing CO_2 from flue gas at a cost lower than that of conventional systems was created and patented in FY12. Developed by researchers at NETL and ADA Environmental Solutions, Inc. (ADA-ES), the BIAS Process was recognized by *R&D Magazine* as among the 100 most technologically significant products introduced into the commercial marketplace within the past year. The sorbent can be used not only in power generation applications but may also be useful in purifying natural gas and converting landfill emissions into fuel.

NETL was recognized as a leader in the development of solid sorbent technology when it was awarded an R&D 100 award.

NETL-RUA research has also resulted in a cheap and effective solution to the problem of capturing CO_2 from gas streams containing hydrogen through the use of modified silicone oil (polydimethysiloxane), a hydrophobic solvent. By altering the molecular structure of the oil so that it cannot cross-link and has a higher solubility for CO_2, a new compound was created, which could someday replace Selexol™ for hydrogen purification and, ultimately, for capturing CO_2 from gasification-based power generation.

Materials and separation technologies developed by the Carbon Capture research team may also impact other areas. For example, NETL patented an epoxy-like resin with CO_2 as one of its ingredients, which may one day take the place of some commercial adhesives. The adhesive sequesters a small amount of CO_2, but its main environmental advantage is that it does not require the use of isocyanate precursors, which are both polluting and toxic. The adhesive may be cured by either light or heat and has generated interest from a major coatings company.

Researchers from the Carbon Capture team worked with collaborators from the Energy Frontier Research Center at the University of California – Berkeley to create the first chemical informatic screening algorithm for ionic liquids. The algorithm allows researchers to quickly screen vast libraries of ionic liquids for important properties such as low viscosity and high CO_2 solubility. The most promising candidates can then be synthesized and tested.

Chemical informatic methods greatly facilitate discovery of new materials in useful—but very large—materials sets like triazolium-based ionic liquids. The first million structures have now been examined and the model fully validated. New ionic liquids with ideal CO_2 capture properties are expected to be synthesized next year.

Another new discovery is an innovative solvent that could improve the process of electroplating aluminum onto iron. This new ionic liquid solvent is non-volatile and does not degrade under process conditions, which gives it a major advantage over existing electroplating technologies that emit hazardous organic pollutants and create coarser aluminum coatings. The new technology may prove useful for creating cheap, corrosion resistant parts for military hardware.

Innovative Process Technologies (IPT)

The NETL-RUA IPT research team 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. These technologies are often at the lower end of the technology readiness scale, but their success would lead to revolutionary changes in the energy market.

The five research tasks being pursued by this team include advanced sensors and controls, power electronics and energetic materials, transformational energy systems, a validation-based computational framework that facilitates the design and development of advanced materials, and improved physics-based computational fluid dynamics (CFDs) predictive capability.

Product gases are sampled from a flat-flame burner, operated with premixed oxy-fuel with steam and CO_2 dilution. The product gases are analyzed using the Raman Gas Composition Analyzer, developed through joint research on an NETL-RUA project with Pitt. The Raman Gas Composition Analyzer can measure all the major product species from combustion, including water vapor, in real time (less than a second).

NETL-RUA IPT research has led to improved computational tools for accelerating the design, development, and deployment of materials for FE applications. The team developed advanced analytical electron microscopy techniques (parallel illumination-nano beam electron diffraction, and electron tomography and three-dimensional reconstruction imaging) that provide materials designers and engineers with important and more accurate information. This information can be used in simulations to predict component service life resulting in better prediction of nano-scale microstructural features that govern the mechanical performance of Fe-9Cr steels.

The team improved multiphase flow modeling in FY12. The performance (speed or time to solution) of NETL's open source multi-phase software, MFIX, was improved by a factor of two through the implementation of a graphics processing unit algorithm neighbor search routine and development of a novel sampling methodology that reduced the number of samples needed for stochastic analysis in uncertainty quantification.

The Convective Disturbance modeling approach was developed for analyzing the dynamic behavior of flames and is improving simulation capabilities for optimizing FE reactors. The Convective Disturbance approach generalizes this behavior, modeling the global flame response by considering the interaction of localized disturbances throughout the steady flame heat release rate distribution. This allows greater flexibility in the model constraints and provides the potential for easy acceptance of inputs of either experimental or steady-state computational flame data.

CCSI

CCSI is a partnership among national laboratories, industry, and academic institutions, including NETL-RUA members, 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, widespread deployment to hundreds of power plants.

On October 10, 2012, the CCSI team released its first set of computational tools and models at its semi-annual Industry Advisory Board Meeting in San Francisco, CA.

This pre-release—which occurred a year ahead of schedule—is a result of intense industry interest in getting early access to these computational tools as well as the phenomenal progress of the CCSI technical team. The initial components of the CCSI Toolset provide new models and computational capabilities that will accelerate the commercial development of carbon capture technologies.

The pre-release consists of new process synthesis and optimization tools 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; and various enabling tools that provide new capabilities such as creating ROMs from reacting multiphase flow simulations and running thousands of process simulations concurrently for optimization and uncertainty quantification.

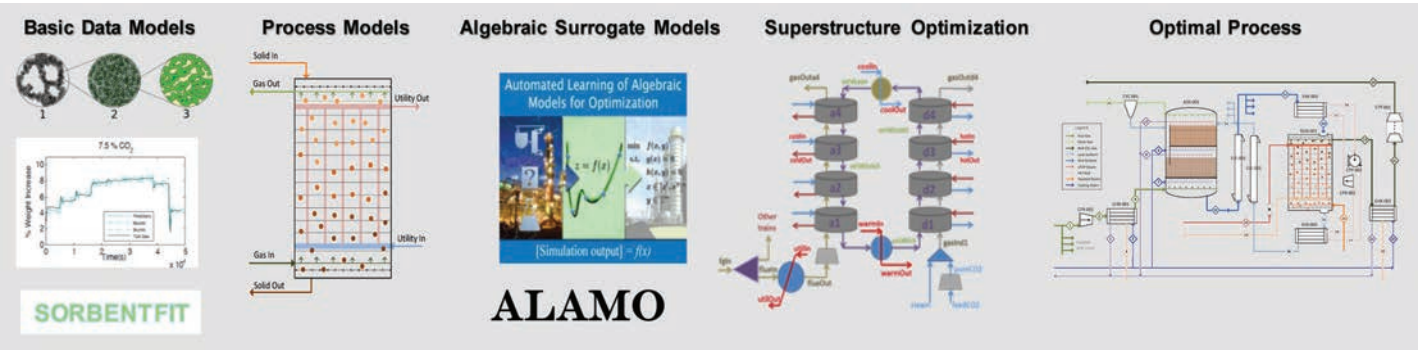
All of the CCSI models can be used within existing simulation tools currently being used by industry. These models will help industry to accelerate development of new carbon capture technologies by (1) enabling new concepts to be rapidly screened using process models, (2) facilitating scale-up by performing detailed equipment simulations using hierarchically validated CFD models, and (3) using these models with other components of the CCSI toolset to optimize equipment and process designs, assess uncertainty, and evaluate risk.

The CCSI toolset will make available models (at various scales) that have a clearly defined validation hierarchy, permitting them to be used to develop different types of carbon capture technologies.

The models will facilitate our ability to understand how uncertainty in input parameters could affect the behavior of the overall physical system. These models will share detailed sub-models of chemical and particle behavior, a feature not found in current models, which will ensure consistency among simulation activities.

Therefore, the Toolset is expected to make significant improvement in how carbon capture systems are developed, providing an approximate 10:1 return on R&D investment and reducing the technology development time by about 25 percent.

Companies that have signed a Test and Evaluation license have begun using these tools and will provide feedback to the technical team to further refine and improve the overall CCSI Toolset. The final release of the completed toolset is planned for January 2016.



The above figure depicts the CCSI Workflow for creating an optimal process using components of the CCSI Toolset. SORBENTFIT was developed by NETL-RUA to create the basic data submodel, which is used inside the CCSI process models. Then, the Automated Learning of Algebraic Models for Optimization (ALAMO) tool, which is being developed NETL-RUA, is used to incorporate the CCSI process models into the CCSI superstructure to determine the optimal process configuration.

National Risk Assessment Partnership (NRAP)

Carbon utilization and storage—the injection of CO_2 into permanent underground and terrestrial storage sites—is an important part of our nation's strategy for managing CO_2 emissions.

Making a business case for large-scale, long-term storage feasibility requires 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 to full-scale carbon storage: long-term liability and cost of monitoring, particularly for post-injection site care.

The NETL-RUA NRAP research team employs core capabilities developed across the DOE's National Laboratory complex to develop tools and methods to quantify risk and reduce uncertainties in order to guide decision-making and risk-management strategies that efficiently achieve DOE's goal of 99 percent CO_2 storage permanence.

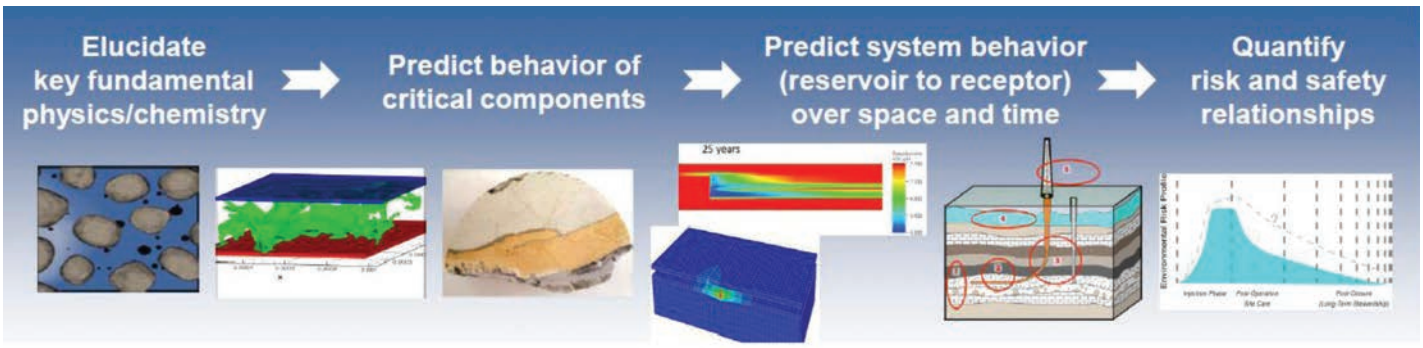
These capabilities are unique within the federal government and can support key decisions and technological solutions tied to many energy challenges, including CO_2 capture, utilization, and storage; shale-gas production; production of deepwater resources; and engineered geothermal systems.

In FY12, the team developed the first ever integrated assessment model (IAM) for carbon storage leakage that includes groundwater impact calculations. This IAM and its upgrades will be used to improve confidence in key storage performance relationships to inform decision-making by operators and regulators. For example, EPA has expressed interest in using NRAP tools to inform upcoming changes in guidance for Class VI well permitting. The IAM can be used for multiple applications such as shale gas, deepwater, and geothermal.

Another concern with drilling and injection operations is the potential for induced seismic events. One of the key recommendations of the recent National Academy of Sciences (NAS) report on seismicity was the creation of a tool to assess induced seismicity.

The NETL-RUA NRAP team performed the first ever probabilistic seismic hazards analysis for induced seismicity related to carbon storage to predict the likelihood and magnitude of a seismic event following storage activities and how it may differ from background seismic activities. Though the current model has limited applicability, subsequent upgrades will extend its scope to more sites. This methodology can also be applied to hydraulic fracturing, wastewater disposal, and geothermal applications.

NETL-RUA has performed laboratory experiments and numerical modeling to assess wellbore cement effects. Results show that standard wellbore cements do not deteriorate significantly in the presence of CO_2, and that chemical reactions between CO_2 and cement may heal defects.



NRAP provides a defensible, science-based methodology and platform for quantifying risk profiles at most types of CO_2 storage sites.

Industrial Carbon Management Initiative (ICMI)

The NETL-RUA ICMI research team is developing carbon management strategies for industrial sources, which are typically smaller sources of 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 on industrial applications, the results are expected to assist in accelerating CO_2 capture technology for coal power generation as well.

Chemical looping combustion (CLC) is a novel method for producing heat or steam from fossil-fueled applications while producing a concentrated CO_2 stream to facilitate carbon capture. Because CO_2 separation is inherent to the process, the cost of carbon capture may be very low, but the process requires high-capacity oxygen carriers.

The NETL-RUA ICMI research team, working with industry, has found a new way to inexpensively manufacture CLC oxygen carriers that have more than twice the capacity for oxygen versus known carriers. These oxygen carriers have (cold) attrition rates comparable to commercial catalytic cracker catalysts and include the addition of a low cost "promoter" to increase oxygen utilization. Two NETL patents were awarded for carrier performance enhancement.

Researchers are currently discussing with industry the use of these carriers in the first pilot-scale demonstration of the concept. In addition to demonstrating CLC, CO_2 enhanced oil recovery and the generation of steam for oil sands recovery may also be integrated in this industrial application.

The ICMI NETL-RUA research team added additional kinetic reaction rates for carrier materials to CFD models resulting in improved prediction of the chemical looping reactor. A chemical looping facility was constructed at NETL to provide benchmarking and validation data for these models. The unit shown above right is currently undergoing shakedown testing and future results will be used for CFD model validation.

Additional ICMI research focuses on the catalytic conversion of captured CO_2 to produce useful chemicals. NETL-RUA researchers developed catalysts that convert CO_2 to chemicals using renewable or waste energy streams for unprecedented electrocatalytic efficiency.

This chemical looping facility at NETL provides experimental data for benchmarking and validation of computational fluid dynamics models.

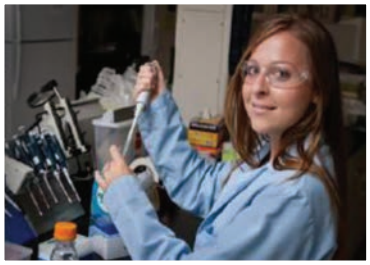
The NETL-RUA ICMI research team has developed unique nanostructured copper catalysts that outperform commercially available catalysts by a factor of ten, and novel metal clusters that have nearly 100 percent electrocatalytic efficiency. The novel metal clusters consist of gold atoms and are a distinct class of nanomaterials that bridge the size gap between molecules and more 'traditional' nanomaterials. They have different non- face-centered-cubic crystal structures and unique electronic structures in comparison to 'traditional' gold nanomaterials. They are 10–100 times more efficient than any other reported technology, have low overpotential that is promising for scalability, and high selectivity that minimizes unwanted side product. A patent for this technology is pending.

Oil and Gas Research

Domestic natural gas and oil resources will continue to play an increasingly critical role in meeting U.S. energy needs provided they can be produced in a manner that effectively addresses environmental concerns (such as air, water, and species protection), as noted in the President's recent executive order on the safe and responsible development of natural gas. The science base needed to support stakeholder decisions stems from the ability to understand the behavior of engineered-natural systems over a range of often extreme conditions.

Under the Energy Policy Act (EPACT) of 2005, NETL 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. This section describes the accomplishments of the NETL-RUA EPACT complementary research program.

A combination of field monitoring, laboratory experimentation and characterization, data mining, and modeling activities are used by NETL-RUA to predict and quantify potential risks associated with oil and gas resources in shale reservoirs.



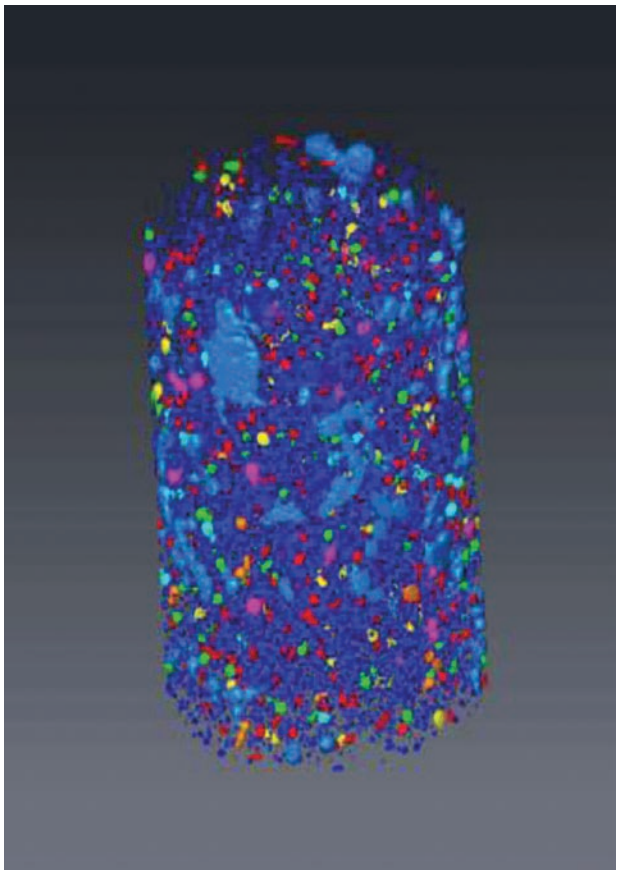
Unconventional Resources

The NETL-RUA Unconventional Resources research team develops 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 these resources. This research requires a combination of field monitoring, laboratory experimentation and characterization, data mining, and modeling activities conducted by an interdisciplinary team comprising federal, contractor, and academic scientists and engineers through NETL-RUA.

In FY12, the NETL-RUA Unconventional Resources research team, using models developed to predict the extent of fracture growth during hydraulic fracturing in target shale reservoirs, was able to demonstrate the infeasibility of hydraulic fractures extending to drinking water aquifers in the Marcellus Shale. The models were verified with field-based microseismic measurements.

The team also made strides in evaluating the influence that wellbores and natural pathways have on gas and fluid leakage. NETL-RUA researchers developed a rapid-throughput analysis technique for analyzing natural tracers (strontium isotopes) as indicators of fluid leakage from shale gas systems. The technique decreases sample analysis time by an order of magnitude compared to conventional testing, reducing processing time from one week to one day. The method is currently undergoing external peer review.

Initiated in FY12, the team spearheaded a public-private collaboration to document environmental baselines and changes resulting from shale-gas development. Data gathered from actual drilling sites before and after commencement of drilling will be used to determine environmental impact.



Researchers study 3-D images of NETL generated foamed cement bubble size distribution (example pictured) to evaluate foam stability under a variety of in-situ conditions.

Ultra-Deepwater (UDW)

As hydrocarbon exploration and production pushes into extreme and often unique environments, the challenges of ensuring safe, low-impact production increase. NETL-ORD's UDW research team is focused on developing a scientific base for predicting and quantifying potential risks associated with exploration and production in extreme offshore environments. The current portfolio of UDW projects spans laboratory-based experimental characterization studies, integration and interpretation of field based datasets, and numerical analysis of the engineered-natural system associated with extreme offshore hydrocarbons.

Several projects in the UDW portfolio are focused on evaluating performance and integrity of key offshore materials for which data in extreme environments are limited. In particular, one UDW project is studying offshore foam cements, for which data on their performance in extreme environments are limited.

Material failures account for nearly two-thirds of all UDW loss-of-control events to date, and these almost entirely align with metallic component failures and deepwater cementing issues. The team collaborated with SwRI to develop baseline "full scale" fatigue properties for the various risers for the five most commonly used offshore alloys. Developing advanced surface treatments for metallic components improves fatigue life as well as general corrosion resistance, thus reducing the likelihood of failure via stress fracturing or corrosion in the field.

The UDW research team used NETL's high-pressure water tunnel facility to determine the impact on rising hydrocarbon gas bubbles under deepwater conditions. Unprecedented images of hydrate-covered gas bubbles were obtained.

The bubble morphology and hydrodynamics are being related to important physical, chemical, and hydrodynamic parameters. This information is needed for accurate deepwater hydrocarbon plume modeling and has provided new data for determining when hydrates could present a problem in a deepwater blowout or around leaking equipment.

Researchers have also provided experimental density data for 20 different hydrocarbons at conditions up to 500°F (260 °C) and 40,000 psi, which have improved the ability to predict hydrocarbon behavior at reservoir conditions.

Expanded drilling in the Gulf of Mexico (and possibly the Arctic) highlights the need for a technology to quickly measure deep sea hydrocarbon leaks. NETL-RUA researchers verified a remotely operated vehicle deployable automatic video analysis technique that can be used to quickly measure deep sea hydrocarbon leaks.

The UDW research team was also the first research group to propose a fluid that successfully satisfies the requirements of a desired "Deepwater Viscosity Standard" and experimentally verify that it exhibits the desired viscosity of 20cP at 500 °F and 35,000 psi.

The first version of an energy data exchange (EDX) was released in July 2012 and is already supporting key NETL R&D portfolios, including the release of the recently updated NATCARB database from the CO_2 Storage program, and the Unconventional Atlas from the EPACT complementary program's unconventional portfolio. In addition, EDX is helping coordinate research and research-driven products associated with NRAP through a newly released NRAP portfolio page.

Increasing Economic Impact

Develop and pursue new business opportunities and funding sources to grow the NETL-RUA research portfolio and capabilities, and leverage core competencies to a broader range of energy and environmental issues and a larger client base.

Growing the Research Portfolio

Expand Funding Resources

NETL-RUA funding in FY12 came almost exclusively from the DOE FE. However, during FY12, NETL-RUA pursued opportunities to diversify funding sources and provide for greater impact of its research capabilities.

NETL-RUA jointly submitted approximately 30 proposals for additional funding for which the results of 14 were announced as of the end of FY12. Distribution of FY12 NETL-RUA joint proposals by lead organization is presented in the chart below left, represented as percentage of proposals.

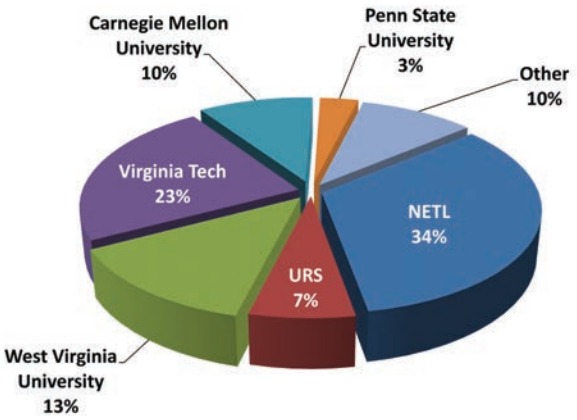
Opportunities being jointly pursued by teams of NETL-RUA researchers tend to be those within other areas of DOE based on the percentage of proposals submitted as shown in the graphic below right.

By the close of FY12, NETL-RUA had won four of the 14 announced awards (12 percent) worth a total of $2.37 million.

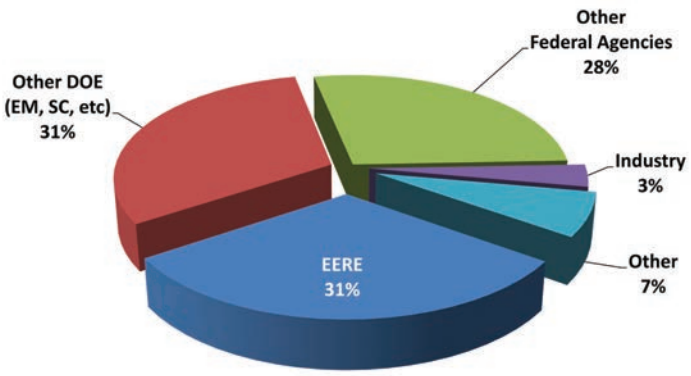
Objectives:

1. Expand NETL-RUA funding resources and research portfolio by successfully pursuing opportunities that leverage the core capabilities, expertise, and activities of the NETL-RUA.
2. Develop strategic partnerships with industry, institutions, other laboratories, and international entities as well as inter-agency in order to obtain access to additional resources.
3. Facilitate the identification, development, and implementation of unique research facilities that can serve as NETL-RUA signature resources.

FY12 Joint NETL-RUA Proposals by Lead Organization



Sources of Funding for FY12 Joint NETL-RUA Proposals



The four joint NETL-RUA proposal efforts that were successful in gaining award funding were the following:

1. Real-Time In-Situ Monitoring and Early Detection of Corrosion Damage in Risers and Structures (Lead: NETL)
2. Electro-deposition of Si anodes for battery applications (Lead: NETL)
3. Expertise in the area of multiphase flow science (Lead: NETL)
4. Advanced Electochemical Materials for Energy Storage Devices (Lead: NETL)

Research award announcements for the balance of NETL-RUA jointly-pursued proposals (with a combined value of $250 million) were pending at the conclusion of FY12.

The proposal work done to date has been noteworthy, particularly the large-scale effort to develop the Energy Innovation Hub – Critical Materials proposal led by Dr. Roe-Hoan Yoon of Virginia Tech. This opportunity, worth approximately $120 million over a five-year period, addresses issues associated with ensuring a stable supply of materials (rare earth elements and others) critical to energy applications. The team submitted a letter of intent in June 2012 and was subsequently invited to submit a full proposal. At the end of FY12, the proposal made the top three, and the applicants were invited for a reverse site visit.

Through developing this proposal, NETL-RUA met a major milestone to jointly pursue, under the NETL-RUA brand, a significant source of R&D funding. This effort also enabled NETL-RUA to learn best practices for undertaking the next endeavor of this magnitude.

Efforts to pursue additional research work through newly developed collaborations are continuing, but lessons learned from the development of the hub proposal indicate that additional infrastructure should be developed to more effectively pursue large-scale research efforts.

Expand Research Portfolio

During the last fiscal year, NETL-RUA spearheaded a strategic push to grow the research portfolio with the introduction of Strategic Growth Areas (SGAs) and associated activities that promoted the NETL-RUA's strategic goals.

This approach to growth was in large part a response to the recognition that the pathway to greater NETL-RUA effectiveness, measured in market acceptance of beneficial new technologies, is to develop energy solutions in conjunction with industry partners. Another was an acknowledgement that continued pressure on the DOE FE budget is expected to limit the available funding from DOE FE for NETL-RUA research in coming years.

FY12 saw the addition of shale gas as an area ripe for new opportunities to team with industry that also aligned well with NETL-RUA skill sets. This brings the total to three initiatives as outlined below.

1. Grid Technologies Collaborative (GTC)
2. Shale Energy Resources Alliance (SERA)
3. Critical Materials Research Alliance (CMRA)

GTC

The GTC's mission is to aggressively engage in research to develop advanced grid-scale power electronics devices and systems for utility-scale high power applications at the transmission and distribution (T&D) levels.

The U.S. electricity transmission system—the Grid—is in need of expansion and updating. Much of the basic design and main infrastructure of the grid is 50 to 100 years old in most parts of the U.S. Improving the performance of the grid is a key component of an NETL-RUA goal to improve energy efficiency, reliability, and power security and for integrating a balanced clean-energy resource portfolio.

The development of models and simulation tools, devices, and systems can contribute to more efficient, secure, and reliable power from coal-based power systems.

Participants in the collaborative include industry partners and researchers from NETL-RUA. The GTC provides the depth of expertise through these partnering organizations for development of power electronics technologies and supporting systems. The GTC engages in three primary activities:

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

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

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. NETL-RUA is leading research on power electronics systems—in the form of both AC and DC applications—that can help to mitigate these effects, facilitating the contribution of these resources to U.S. electricity generation.

In FY12, the GTC initiated its collaborative research effort to assess the technological advances necessary to bolster power delivery capability from offshore to onshore, making it a feasible economic value proposition.

Working as a team, researchers from NETL-RUA provide systems-level modeling, simulation, and analyses capabilities combined with experience in grid infrastructure technologies and key components.

The first phase of the collaborative research effort focused primarily on modeling and simulation to develop validated steady state and dynamic models of system interactions at the converter-grid interface, including consideration of a next generation power converter. This effort concluded with the understanding that the converter development going forward will be established as a scalable bi-directional three-phase AC-DC interface for utility-scale high power applications at the T&D levels.

The GTC furthers the commercialization of the technologies it develops by working closely with industry, building off established relationships with the partner universities, and engaging all relevant constituents engaged in the chain of power electronics development and application. Industry partners bring real-world perspective to the R&D activities of the GTC.

SERA

The Shale Gas SGA team is focused on developing solutions for shale gas technology challenges and science-based resources for decision-making and general knowledge.

Rapid development of the Marcellus Shale over the past few years has led to a number of technology needs related to sustainable development of the shale gas resource, and concerns regarding the potential effects of shale gas development on human health and the environment.

To respond to these issues, the Shale Gas SGA team established SERA to conduct research on key areas related to shale energy development, demonstrate technologies supporting the environmentally sustainable development of shale energy resources, serve as a repository of data regarding shale energy resources and environmental effects, and promote dialogue among stakeholders.

SERA plans to initially focus on research in the following three areas:

- Air Emissions: Research will be conducted to advance the state-of-the-art in regional air quality modeling and lifecycle GHG assessment as it relates to development of shale gas resources.
- Shallow Stray Gas: Research will be conducted to evaluate whether naturally forming gas can affect groundwater aquifers, detect gas migration along wellbores, and determine solutions for preventing gas flow in wellbore from shallow gas formations.
- Water Sourcing and Disposal: SERA will serve as a single resource to evaluate the costs and performance of various water management options for the shale energy sector. While many treatment technologies are available on the market, there are many that are unproven in the shale gas context.

The SERA business plan was presented to the NETL-RUA EC in November and is anticipated to be approved and funded in early 2013.

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

CMRA

Established in FY11, the CMRA focused much of this past year responding to DOE's Energy Innovation Hub – Critical Materials solicitation. As such, it is the first SGA team to make a major play toward self-sustainability.

Energy Innovation Hubs are part of the Obama Administration's broad-based, clean energy research strategy to harness American innovation. This strategy is focused on needed breakthroughs in important technologies to grow the clean energy economy and generate new, clean energy jobs.

The Critical Materials Energy Innovation Hub will address challenges related to critical materials, including mineral processing, manufacture, substitution, efficient use, and end-of-life recycling; integrate scientific research, engineering innovation, manufacturing, and process improvements; and find a holistic solution to the materials challenges facing the nation.

The requirements of the hub solicitation matched well with CMRA's mission to:

- Develop technologies that enable the exploitation of diverse critical material supply sources.
- Develop a portfolio of viable technologies that reinvigorates domestic industry and U.S. technological competitiveness.
- Perform research at all stages of technology advancement to discover groundbreaking technology.
- Develop flexible technologies that use critical materials more efficiently, use less of them, or avoid their use altogether.
- Emphasize commercialization from concept onward by vertically integrating research activities to promote investment.

The partnerships fostered during the development of this proposal are providing opportunities to pursue work with industry, and the team continues to pursue other options.

Develop Strategic Partnerships

Teamwork is a hallmark of the collaboration, and relationship building will continue to pave the way for joint scientific research ventures and future success.

Numerous university work collaborations are occurring between investigators who have cultivated relationships through their NETL-RUA contacts. Some highlights of these inter-university efforts are as follows:

Teaming arrangements among Penn State, Virginia Tech, and WVU have enhanced the ability of these NETL-RUA universities to win awards from the U.S. Department of Transportation as well as the U.S. Department of Agriculture (USDA) for work such as the "Mid Atlantic Universities Transportation Center" and "Refining and Harmonizing Phosphorus Indices in the Chesapeake Bay Region to Improve Critical Source Area Identification and to Address Nutrient Management Priorities" respectively.

Penn State and CMU teamed to win an award for work with the Air Force Office of Scientific Research. The project was entitled "Algebraic Studies for Network Models."

Penn State and WVU combined their efforts to win a USDA award for the "Northeast Woody/Warm-Season Biomass Consortium."

Researchers from Pitt and WVU created a winning proposal entitled "Computational Design of Metal Organic Frameworks for Photocatalytic Reduction of CO_2." The award was provided by the Basic Energy Sciences program of the Office of Science on behalf of the DOE.

A significant NETL-RUA success is the receipt of a Richard King Mellon Foundation grant of $22 million to the Center for Energy within Pitt's Swanson School of Engineering. Award of this grant, one of the largest private foundation grants in its history, was due in part to Pitt's teaming arrangement with NETL-RUA.

The grant will serve to accelerate the research and education efforts of Pitt's Center for Energy, which is dedicated to improving energy technology development and sustainability through the work of more than 70 world-class faculty members and their research teams, some of which are also engaged with NETL-RUA.

"With this funding, we will be in a much better position to attract top-notch faculty and students to our region. This will advance our creative and productive partnerships with regional and national companies, and with national laboratories, particularly with our region's National Energy Technology Laboratory."

—Brian Gleeson, University of Pittsburgh NETL-RUA Consortium Area Lead and Center for Energy Director, commenting on the Richard King Mellon Foundation grant.

In addition to the collaborative arrangements that led to numerous successful joint awards, individual efforts from Alliance members led to awards for energy research from prestigious agencies and organizations such as the Heinz Endowments, National Science Foundation, and the Stanford Global Climate & Energy Project. Combined, these efforts have led to an overall influx of grant and contract awards in excess of $31.6 million to NETL-RUA member universities.

These winning efforts are indicative of the teaming arrangements within the NETL-RUA and provide the promise of greater things to come in the collaboration.

Develop NETL-RUA Signature Resources

Simulation-Based Engineering User Center (SBEUC)

On September 16, 2010, DOE Secretary Steven Chu announced the creation of the SBEUC located at NETL. Funded with $20 million from the American Recovery and Reinvestment Act, the SBEUC will be used primarily for developing and deploying the simulation tools to accelerate the R&D of carbon capture and sequestration technologies and support the Administration's goal to overcome the barriers to widespread, cost-effective deployment of carbon capture and storage within 10 years.

A high-performance computer will allow researchers to simulate phenomena that are difficult or impossible to investigate experimentally. The results from simulations will become accessible through user centers that provide advanced visualization capabilities and foster collaboration among researchers.

An eagerly anticipated suite of 21 computational tools and models to help enable rapid development and deployment of new carbon capture technologies became available from the CCSI in 2012.

The toolset developed by CCSI (a public-private partnership led by FE) will help meet an urgent industry need to take carbon capture concepts from the laboratory to the power plant more quickly, at lower cost, and with reduced risk. It works with commercial and open-source software currently in use by industry and includes new, highly versatile software tools developed to fill technology gaps.

In addition to helping with carbon capture technologies, the tools can be used to accelerate technology development for refining, chemicals production, and oil and natural gas production. The SBEUC will be accessible to researchers at other DOE National Laboratories as well all NETL-RUA member organizations.

The SBEUC is the newest facility in NETL-RUA's portfolio of signature resources, which includes AVESTAR™, NETL-Morgantown and WVU Center; the Penn State Advanced Turbine Laboratory; and the NETL-RUA Isotope Analysis Facility at Pitt.

The image above is the Morgantown Visualization Center which allows collaborative research between NETL sites and RUA partners through remote sharing of large data sets and images among researchers.

NETL's High-Performance Computer for Energy and the Environment located at NETL's SBEUC allows collaborative research between NETL sites and NETL-RUA partners through remote sharing of large data sets and images among researchers.

Accelerating Innovative Solutions

Facilitate the management, dissemination, and commercialization of the intellectual assets created through NETL-RUA by leveraging its combined knowledge, experience, networks, and best practices to support energy innovation and entrepreneurship to stimulate economic growth.

Intellectual Property

Identify and Facilitate Conversion of Intellectual Assets into New Products, Processes, and Jobs

NETL-RUA accomplishments within the intellectual property domain include 24 patent disclosures and the filing of two provisional patent applications. A significant increase in the number of patents issued in FY12 is one indication that the collaboration is providing increased innovation. For a more inclusive look at the global NETL Intellectual Property Statistics for FY10, FY11, and FY12 see the following table.

NETL FY2010, FY2011, and FY2012 Intellectual Property Statistics

Intellectual Property Management	FY2010	FY2011	FY2012
Inventions Disclosed	30	17	24
Total Inventions Reviewed	13	20	19
Provisional Patent Applications	4	3	2
Non-Provisional Applications	12	9	13
All Patent Applications	16	12	15
Patents Issued	6	4	12

The following narrative highlights some of the patented inventions resulting from NETL-RUA research.

Objectives:

1. Promote, facilitate, and forge partnerships to convert intellectual assets into new products, processes, and jobs.
2. Share best practices of the NETL-RUA organization members to aid in the development of processes and agreements that advance the technology transfer mission.
3. Identify potential intellectual assets resulting from NETL-RUA research projects and optimize their value.

Laser-Induced Breakdown Spectroscopy (LIBS) for Real-time Compositional Analysis:

On August 6, 2012, the world watched the Curiosity rover land on the surface of Mars. The rover, in addition to carrying sophisticated detection devices, was equipped with a LIBS instrument called ChemCam.

LIBS is a laser-based analytical technique that provides rapid elemental and isotopic analysis of solid, liquid, and gas samples. Within ChemCam, the LIBS system is coupled with Raman spectroscopy to analyze molecular species. ChemCam was fabricated at Los Alamos National Laboratory where NETL-RUA members had the opportunity to view the unit prior to its shipment to NASA.

LIBS is a versatile measurement technique that can be applied to multiple measurement modalities and simply needs some engineering and refinement to become a highly useful portable system for routine, widespread monitoring. NETL-RUA researchers are using LIBS for carbon sequestration monitoring and measurement.

This setup essentially comprises a high intensity laser as an excitation source and a time-gated spectrometer to collect the signal. A laser beam is focused onto a solid sample or within a gaseous or liquid sample to create high temperatures, dissociating the sample to form plasma. Radiation from the plasma is then collected by the spectrometer.

Subsequent analysis of the radiation gives qualitative and quantitative information of chemical elements present in the sample.

The technique's versatility has also allowed NETL researchers to use LIBS for developing calibration standards to aid CT scanning technology. This work won a best paper award from the Society of Petroleum Engineers in Denver, Colorado.

The application of LIBS in carbon sequestration research led NETL to submit a patent disclosure for developing a sensor to perform real-time measurements in the field. This sensor applies the laser spark plug technology that was developed at NETL and featured in the article "Laser Car Ignition Dream Sparks Multiple Approaches," in the September issue of *Photonic Spectra*.

In the remote sensing application, the system would allow for a centrally located computer/controller to connect to multiple sensor locations instead of deploying many LIBS analysis systems to multiple locations.

This development will allow NETL researchers to apply the LIBS technique to a number of carbon sequestration and Marcellus Shale research projects such as CO_2 leak monitoring, seal integrity, CO_2-rock interaction, and Marcellus shale gas and water monitoring.

Improving Lithium-Ion (Li-ion) Battery Performance

Li-ion batteries are one of the most popular types of rechargeable batteries with one of the best energy densities, no memory effect, and a minimal loss of charge when not in use.

Li-ion batteries have also grown in popularity for military, electric vehicle, and aerospace applications. It is becoming increasingly important to develop batteries with higher energy density, good cyclability, and fast recharge capability in order to meet the escalating demands of energy storage device applications like smart grid energy and electric vehicles.

A 2 x 28 volt, 30Ah lithium ion battery designed for the Mars Rover.

Graphite is currently the preferred anode used in Li-ion based battery systems. Amorphous silicon (a-Si) films are an attractive alternative to graphite as an anode material because they can provide a four- to five-fold increase in storage capacity. Additionally, a-Si exhibits excellent stability over hundreds of charge-discharge cycles—another desirable feature for a rechargeable battery.

NETL and Pitt have teamed on research funded by DOE's Office of Energy Efficiency and Renewable Energy that has resulted in a novel, low-cost approach for depositing a-Si for Li-ion battery anodes, which will improve the performance of the batteries in transportation applications such as hybrid plug-in and electric vehicles.

The team has devised a simple electroplating technique to deposit a-Si films directly on copper foils, which could then be immediately assembled as an anode in a Li-ion battery pack.

This technique has the potential to save considerable time and reduce processing costs by eliminating intermediate processes in traditional battery manufacturing.

A joint patent application has been filed for the technique, and results of the research have been published in *Materials Science and Engineering: B*.

NETL Patent Addresses Catalyst Deactivation, Diesel Reformation

When NETL researchers patented a unique hexaaluminate catalyst, they made significant progress toward solving a problem associated with catalyst deactivation—one that had long inhibited processes such as diesel fuel reforming.

Researchers have long wrestled with the problem of commercially available catalysts deactivating in the presence of sulfur and aromatic compounds in diesel fuel. Researchers needed to find a solution to the deactivation problem in order to successfully convert diesel fuel into synthesis gas—a process known as reforming.

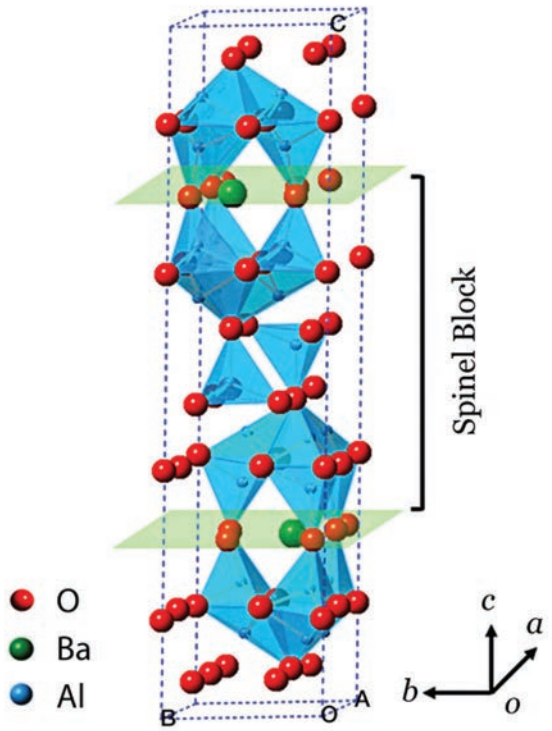
NETL researchers developed a method to reform hydrocarbon fuels using hexaaluminate catalysts. The method successfully disrupts the formation of carbon that leads to the deactivation of the catalysts, a key element in the reforming of hydrocarbon fuels, and minimizes deactivation under the most severe reforming conditions.

The technology behind the NETL patent entitled "Methods of Reforming Hydrocarbon Fuels Using Hexaaluminate Catalysts," works by using the unique unit cell structure of the hexaaluminate oxide compound as a molecular scaffold to atomically disperse and support catalytically active metals. By doing so, the active metals are maintained in a state of low coordination to disrupt the carbon formation. A series of articles (Gardner et al., *J. Phy. Chem.* C 114, 2010, 7888-7894 and *Catalysis Today* 157, 2010, 166-169) describes the unique structural characteristics and catalytic properties of the materials.

The technology could be applied, for example, to the trucking industry where hydrogen needed for fuel in SOFCs can be produced by converting the hydrocarbons present in long-haul truck diesel fuel into synthesis gas.

Nationwide, 2.2 million long-haul trucks produce an estimated 11 million tons of CO_2, 200,000 tons of nitric oxide, and 5,000 tons of particulate matter annually. The trucks waste more than 1 billion gallons of diesel fuel while idling. By incorporating SOFCs, these trucks could obtain power from a cleaner, more efficient power source.

The technology is available from NETL for licensing and/or further collaborative research. The technology could potentially compete with conventional methane reforming catalyst technology, and it is useful for dry reforming, partial oxidation, and steam reforming applications.



Hexaaluminate's unique cell structure acts as molecular scaffold for catalytic metals that disrupt formation of carbon. Carbon formation is not desired as it leads to catalyst deactivation.

SPECTRALINE

Preparing Tomorrow's Energy Leaders

Create a culture of energy leadership through promotion of education and entrepreneurship.

Creating Energy Leaders

There is an increasingly critical need for multi-stakeholder partnerships to provide knowledge, expertise, mentoring, and financial support to educate the next generation of energy leaders.

NETL-RUA, through its research and educational programs, links various stakeholders for collaboration in mentoring young professionals to prepare them to perform innovative research and transfer new technologies to the marketplace.

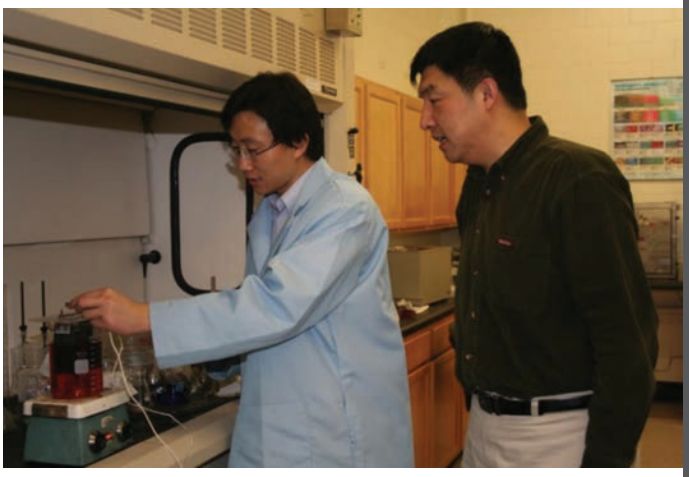
Research that has not been sufficiently explored in the market presents opportunities for students to pursue new venture projects. To facilitate such ventures and product development, NETL-RUA provides laboratory space, time, and collaboration opportunities with faculty and business partners.

		2010	2011	2012
NETL-RUA Student Researchers		107	133	115
Advanced Degrees Conferred	Ph.D.	20	20	23
	Masters	13	8	18

In FY12, students participated on 65 percent of NETL-RUA projects. In addition, 102 students obtained advanced degrees from 2010 to 2012 while working on NETL-RUA-funded research efforts. Over 100 students, including undergraduates, are involved in NETL-RUA research annually.

Objectives:

1. Establish collaborative energy education programs within the NETL-RUA using the research as a springboard.
2. Facilitate the exchange of personnel among NETL-RUA organizations.



NETL-RUA partnerships encourage future generations to maintain U.S. leadership in the energy industry. From left, WVU graduate student, Junwei Wu, and Associate Professor of Mechanical and Aerospace Engineering, Xingbo Liu.

Spotlight on Student Achievements

Peilin Cao Passes Ph.D. Qualifying Exam While Performing Wellbore Integrity Research

NETL-RUA graduate student, Peilin Cao

NETL-RUA graduate student, Peilin Cao, is a Ph.D. candidate at Penn State.

Her thesis, entitled "Experimental Investigation of Conditions Affecting Wellbore Integrity due to Chemical Reaction using X-Ray Micro-CT Imaging" examines the property evolution of wellbore cement as well as its integrity when exposed to CO_2-rich brine under geological sequestration conditions.

Cao has worked with Penn State Professor Zuleima Karpyn on the wellbore integrity project as part of NETL-RUA's Carbon Storage research team since spring 2011.

Cao passed her Ph.D. comprehensive exam in September 2012, presented one poster at the 2012 fall meeting of the American Geophysics Union in December, and is also the primary author on a submitted journal article.

Richard Alesi Completes Ph.D. with Dissertation on Amine-based Sorbents

NETL-RUA graduate student, W. Richard Alesi

NETL-RUA graduate student, W. Richard Alesi, completed his Ph.D. and graduated from the Chemical Engineering department of CMU in 2012.

His dissertation was entitled "Amine based sorbents: Developing a quantitative framework for understanding CO_2 capture." Alesi was advised by Professor John Kitchin of the Department of Chemical Engineering at CMU.

Alesi worked on several projects related to the development and characterization of CO_2 capture sorbents with NETL-RUA's Carbon Capture research team. His most recent work was the characterization of the CO_2 capture performance of a commercially available ion exchange resin containing primary amines.

He found this material had moderate capture capacity and superior moisture resistance compared to other materials currently being investigated. Alesi published two papers and gave twelve different presentations on his work.

Justin Beck Successfully Defends Dissertation on Corrosion in Supercritical CO_2 Environments

NETL-RUA graduate student, Justin Beck

Justin Beck received his Ph.D. from Penn State in October 2012 after defending his dissertation as part of the NETL-RUA Carbon Capture research team project. The title of the dissertation was "Electrochemical Measurements of Corrosion in Supercritical CO_2 Environments."

The project focused on the development and testing of a corrosion probe capable of performing electrochemical measurements in a bulk supercritical CO_2 phase contaminated with water vapor, which was achieved by coating the probe surface with a layer of ion-conductive polymer.

The work was completed under Serguei Lvov, a professor of Energy and Mineral Engineering and Materials Science and Engineering, and Director of the Electrochemical Technologies Program at the Earth and Mineral Sciences (EMS) Energy Institute at Penn State. The research was performed as a joint venture between the EMS Energy Institute at Penn State and NETL-Albany. In addition to the dissertation, Beck prepared four conference transaction papers on the research results and personally presented his work at the 2012 Electrochemical Society Conference.

Tetsuya Kaneko Completes Ph.D. on the Study of Gasifier Refractory Degradation

NETL-RUA graduate student, Tetsuya Kenneth Kaneko

NETL-RUA graduate student, Tetsuya Kenneth Kaneko, successfully defended his Ph.D. dissertation at CMU in May 2012.

His thesis entitled "Effects of Temperature, Oxygen Partial Pressure, and Materials Selection on Slag Infiltration into Porous Refractories for Entrained-Flow Slagging Gasifiers" examined the relationship between refractory degradation and a number of other varying gasification parameters.

Kaneko worked with CMU Professor Sridhar Seetharaman on the slagging gasifier project as part of NETL-RUA's Advanced Gasification research team. With the help of his group, he contributed two posters, one conference presentation, and is the primary author of three journal articles.

Thesis committees are composed of personnel from wide ranging organizations and are designed to provide the best experts for research project review. Peter Rozelle of DOE FE Headquarters was one of the experts on Kaneko's thesis committee.

Job Kasule Successfully Defends Ph.D. Thesis on Simulating Entrained Flow Gasification

NETL-RUA graduate student, Job Kasule

NETL-RUA graduate student, Job Kasule, successfully defended his Ph.D. dissertation at WVU in September 2012.

His thesis entitled "Mathematical Modeling and Simulation of a 1-D Transient Entrained flow GEE-Texaco Coal Gasifier" focused on the use of simulation tools such as Aspen Custom Modeler® to model and simulate the performance of an entrained flow type gasifier for use in a plant-wide IGCC Plant model.

Kasule worked with WVU Professors Richard Turton and Debangsu Bhattacharyya from the Department of Chemical Engineering on this project to develop an entrained gasifier model as part of NETL-RUA's Advanced Gasification research team. Kasule also contributed six podium papers at the following meetings: the Annual American Institute of Chemical Engineers (AIChE) Meeting, Pittsburgh International Coal Conference, and the West Virginia Academy of Science 2010 meeting.

He is the primary author of a recently published journal article entitled "Mathematical Modeling of a Single-Stage, Downward-Firing, Entrained-Flow Gasifier." He is also in the process of submitting another journal article entitled "On the Transient modeling of an Entrained-Flow Gasifier using Aspen Custom Modeler." He is currently a post-doctoral fellow in the Department of Chemical Engineering at WVU.

Stephen Zitney of NETL's Process and Dynamic Systems Research Division represented NETL on his thesis committee.

Juan Ma Receives Masters Degree for Her Work on Mineralization of CO_2 for Carbon Storage

NETL-RUA graduate student, Juan Ma

NETL-RUA graduate student, Juan Ma successfully defended her Masters thesis at Virginia Tech in April 2012.

Her thesis entitled "CO_2 Mineralization Using Reactive Species" explored the possibilities of mineralizing CO_2 with reactive species such as magnesium ions and calcium ions present in nature such as in sea water.

Ma worked with Virginia Tech Professor Roe-Hoan Yoon on the mineralization of CO_2 as a carbon capture and storage option. She served on the 2011 CO_2 Water Rock Geochemistry research team.

She presented her results at the 2012 AIChE Annual Meeting, and is the primary author of a journal article that will be submitted in 2013.

Matthew Payne Passes Ph.D. Qualifying Exam and Will Study Advanced Alloy Designs

NETL-RUA graduate student, Matthew Payne

NETL-RUA graduate student, Mathew Payne, successfully passed his Ph.D. qualifying exam in Chemical Engineering at CMU during 2012. Payne joined the Ph.D. program at CMU after having completed a Bachelor of Science in Chemical Engineering from WVU in the spring of 2011.

Payne will be working on a project under the NETL-RUA IPT research team entitled "The oxidation kinetics of AlxFeyNi1-x-y alloys studied across composition space." He will be using high throughput methods to grow composition spread alloy films of these three components such that the film contains all possible compositions of the ternary alloy. This is coupled with study of the oxidation kinetics using high throughput methods to measure oxide growth across all alloy compositions.

Payne works with Professors Andrew Gellman and James Miller in the Department of Chemical Engineering at CMU. His project is part of a much larger NETL-RUA effort to develop advanced computational and experimental methods to predict the properties of complex materials such as alloys and to accelerate the design of new alloy materials.

Chris Purcell Successfully Defends Ph.D. Dissertation for His Work on Rock Physics Response to CO_2 Injection

NETL-RUA graduate student, Chris Purcell

NETL-RUA graduate student, Chris Purcell, successfully defended his Ph.D. dissertation at Pitt in June 2012.

His thesis entitled "Velocity Measurements in Reservoir Rock Samples from a Limestone Unit Using Various Pore Fluids, and Integration with Well Logs and Seismic Data" studied the response of rock physics properties on core samples to CO_2 injection as part of a carbon sequestration project in West Texas.

Purcell worked on this carbon sequestration project with Pitt Professor William Harbert of NETL-RUA's Carbon Storage research team, Igor Haljasmaa of URS, and Yee Soong of NETL's Geosciences Division at NETL's Core Flow Laboratory. He also contributed posters, papers, and talks at various conferences.

NETL-RUA encourages multi-organizational thesis committees to provide the best experts for the research review. As an example of this, Soong represented NETL on his thesis committee.

Chris is currently working for Nexen Inc. in Houston, Texas, as a geophysicist and continues his interactions with industry and academic research groups.

Collaborative Energy Education Programs

NETL-RUA Business and Entrepreneur Workforce Development

NETL-RUA members are working with business schools to incorporate NETL-RUA projects into their business plan coursework. The strategy behind setting up these partnerships is three-fold.

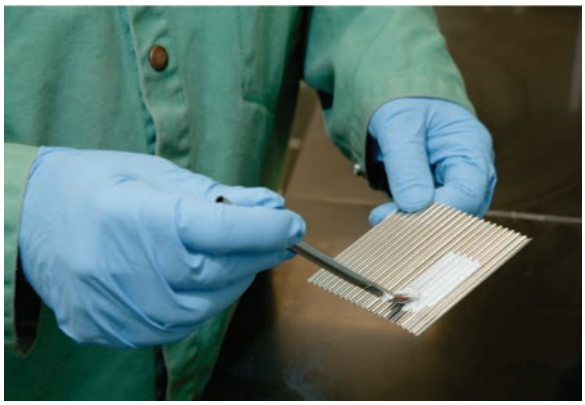
1. Business schools have students that are entrepreneurial in nature. A business student may want to spin-off a company based on an NETL-RUA technology.
2. The students are providing business development support with the only expense being the time invested by an NETL-RUA researcher to provide the students with technology background information. As a result, NETL receives at minimum a report presenting various technology commercialization scenarios.
3. Interactions with the business schools provide added visibility for NETL-RUA by creating partnerships outside of NETL's traditional contacts in the university engineering schools

In 2011, NETL-RUA researchers began a partnership with the University of Oregon's Lundquist Center for Entrepreneurship to provide opportunities for graduate students pursuing an MBA who are interested in the commercialization of new technologies.

The partnership has continued with students, NETL-RUA researchers, and NETL's Technology Transfer Group working together on select NETL-RUA inventions to study and promote new technologies in academic and industrial settings. Technology and business feasibility assessments, business plan development, and internal and external competitions are all part of the entrepreneurship process as these MBA students collaborate with NETL-RUA researchers.

One such project has had significant success in national and international business plan competitions, and has led to the formation of the start-up company, Corrosion Solutions.

This company is based around NETL's patented R&D 100 award-winning cerium oxide coating for metallic alloys. This coating can be applied to metals by brushing, spraying, or dipping, and helps to increase the oxidation resistance of Ni-based superalloys, as well as ferritic and austentic stainless steels, by diffusing into the metals. This technology improved metal oxidation resistance and can be applied easily and inexpensively.



Cerium oxide-based coating

Personnel at Corrosion Solutions are currently securing a license from NETL to market the cerium oxide coating and creating business plans to target the high-end barbeque grill market. After entering this market, the company has plans to further market the coating for power plant applications.

In another example, NETL-RUA worked with Pitt's Joseph M. Katz Graduate School of Business to arrange meetings between its entrepreneurs and NETL-RUA researchers to discuss potential technologies to commercialize. The students worked in teams to develop business development concepts.

NETL has received two commercialization plans thus far for its High Capacity Immobilized Amine Sorbent and its Poly (Hydroxyl Urethane) Adhesive as a result of this effort.

In FY13, NETL-RUA plans to establish similar connections with the business school programs of its other university partners.

Personnel Exchange

Researchers regularly access NETL campus locations. Researchers that visit on a regular basis (at least three times per week) to perform research and attend meetings are picture-badged for access.

A total of 35 faculty members were badged for access to NETL (20 for NETL-Pittsburgh and 15 for NETL-Morgantown) during FY12. This includes all CALs, Principal Investigators (PIs), Co-PIs, and faculty that visit NETL on a regular basis.

A total of 51 additional NETL-RUA members are picture-badged for access to NETL (23 for NETL-Pittsburgh and 28 for NETL-Morgantown). This includes all graduate students, undergraduate students, post docs, and other researchers visiting NETL on a regular basis.

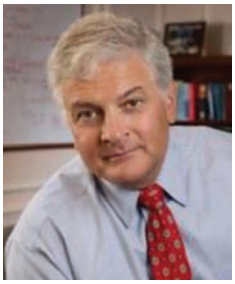
NETL researchers have also served as adjunct faculty for a number of member university courses, including participation on thesis and dissertation committees.

NETL researchers have been participating as faculty and technical presenters within NETL-RUA in an effort to increase reciprocal researcher relationships and provide students with access to subject matter experts.

A total of 36,160 hours of university faculty research were completed onsite at NETL in 2012. Ten NETL ORD employees are currently serving as adjunct professors at NETL-RUA universities.

Operations

FY2012 NETL-RUA Executive Committee



Henry Foley

Vice President for Research,
Pennsylvania State University

Terri Marts

Vice President and
Program General Manager,
URS Corporation

Andrew Gellman

Co-Director,
Wilton E. Scott Institute for
Energy Innovation,
Carnegie Mellon University

Cynthia Powell
(Committee Chair)

Director, Office of Research
and Development,
National Energy Technology Laboratory

Julianne Klara

NETL-RUA Manager,
National Energy Technology Laboratory

Mark Redfern

Vice Provost for Research,
University of Pittsburgh

Fred King

Associate Dean for Research
and Graduate Studies,
West Virginia University

Christina Gabriel
(ex officio)

President
University Energy Partnership

William Knocke

Associate Vice President
for Research Programs.
Virginia Polytechnic Institute
and State University

NETL-RUA
Regional University Alliance

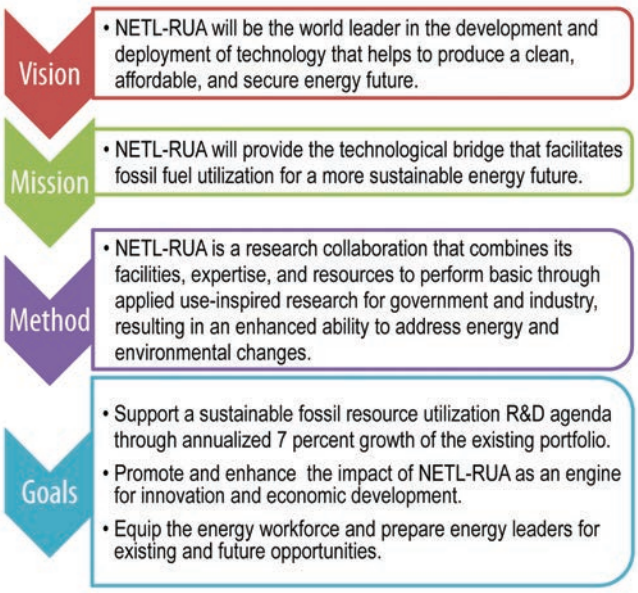
NETL-RUA at a Glance

NETL-RUA's structure and operational processes continue to evolve. The initial governance structure based on an EC still stands. However, NETL-RUA's EC decided to dissolve the standing committees in favor of a more flexible set of ad hoc teams that will be chartered to accomplish specific tasks comprising the EC's strategic planning effort.

In FY12, the EC revisited NETL-RUA's vision, mission, and goals in order to provide additional strategic and executive guidance to its membership.

The strategic planning session resulted in definition of a long-term vision for the Alliance and development of near-term goals for increasing the visibility, impact, and size of the NETL-RUA's R&D portfolio.

The graphic below illustrates the cornerstones of the strategic plan. Strategies and actions to successfully achieve the stated goals are being developed, and the strategic plan is expected to be implemented in early 2013.

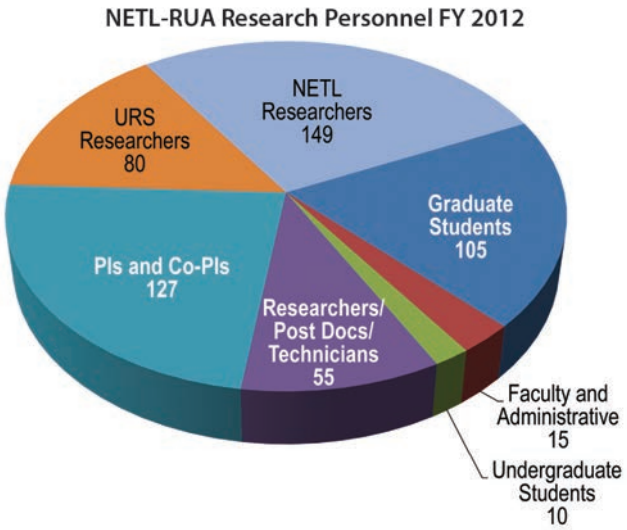


Resources

NETL-RUA researchers are federal scientists, engineers, and interns from NETL/ORD; faculty and students from the universities; and researchers from URS resulting in a collective staff of over 500 researchers.

University Researchers	URS Researchers	NETL Researchers	Total NETL-RUA Researchers
312	80	149	541

The distribution of faculty, post-docs, and students is presented in the pie chart below.



These researchers are engineers, chemists, materials scientists, geologists, computer specialists, and personnel working in other scientific disciplines, many of whom are recognized as leading experts in their fields.

There is continued emphasis on involving graduate and undergraduate students in research activities to encourage continuing education in science and technology and create the next generation of engineers and scientists who will understand the energy challenges facing our nation and the world.

Outreach and Impact

Increase the visibility and impact of NETL-RUA R&D as evidenced by contributions that affect a broad range of energy-related issues and through outside recognition for exceptional research efforts.

Advancing the Impact of NETL-RUA Research

External Outreach

2nd Annual NETL-RUA Energy and Innovation (E&I) Conference: The conference was held November 28–29, 2012, at the Southpointe Hilton Garden Inn in Canonsburg, Pennsylvania, and attracted nearly 200 business and industry leaders from Pennsylvania, West Virginia, Ohio, and Virginia as well as NETL-RUA members.

NETL-RUA hosted the event in collaboration with Catalyst Connection to highlight, demonstrate, and exhibit NETL-RUA research capabilities to the region's manufacturing sector and facilitate the development of new partnerships that will be instrumental in future collaborative research and economic development.

The two-day conference featured keynote addresses by area business and industry leaders, informational tracks, and networking, matchmaking, and poster sessions featuring NETL-RUA researchers.

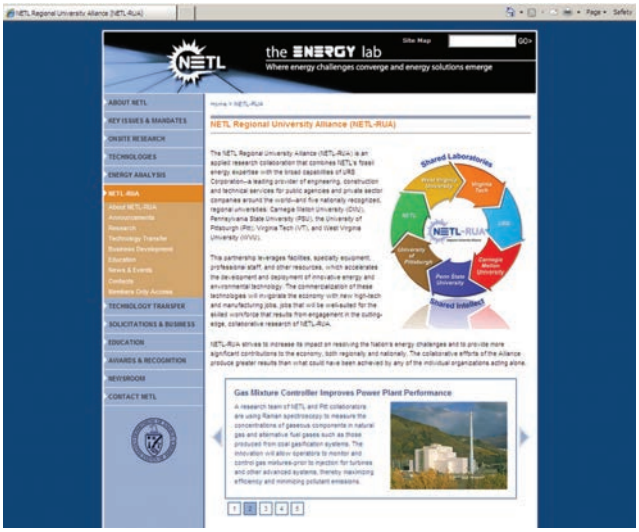
The conference provided a significant opportunity for researchers to promote the collective capabilities of NETL-RUA to the region's manufacturing sector, thus improving the visibility of NETL-RUA as a powerful vehicle to drive innovation in energy and environmental research and serve as an R&D resource for the region's manufacturing industry.

Video of all conference speakers, posters, technical presentations, and innovation success stories are available for viewing at http://www.netl.doe.gov/rua/events.html on the NETL-RUA website.

Objectives:

1. Inform a diverse audience of the mission, importance, impacts, and successes of the NETL-RUA
2. Facilitate communication and sharing of information among NETL-RUA membership
3. Develop tools and materials that will assist NETL-RUA membership in championing the NETL-RUA

2nd Annual NETL-RUA E&I Conference Attendees



NETL-RUA External Website

NETL-RUA Website: The NETL-RUA website, hosted on the NETL website at http://www.netl.doe.gov/rua/aboutrua.html, continues to serve as the key informational source for NETL-RUA's history, mission, member organizations, and reference information such as fact sheets and reports. News and events, contact information, and a members-only area are also integrated into the website.

While this website was initially designed to provide NETL-RUA members with an information portal, it is being redesigned in its second year of existence to provide up-to-date information on facilities, researchers, capabilities, and products.

The new website will be targeted at cultivating new partners and strengthening ties with existing ones, and also focus on SGAs in which NETL-RUA researchers are working to expand their engagement with industry. The updated NETL-RUA website will be unveiled in spring 2013.

NETL-RUA Public Fact Sheet: As NETL-RUA programs continued into their second full year, the NETL-RUA public fact sheet became due for an update.

The new fact sheet presents an updated overview, objectives, and key contacts of the program, as well as highlighted partnerships, key research, and latest awards presented to the NETL-RUA. The fact sheet can be viewed on the NETL website at http://netl.doe.gov/rua/aboutrua.html.

NETL-RUA Public Fact Sheet

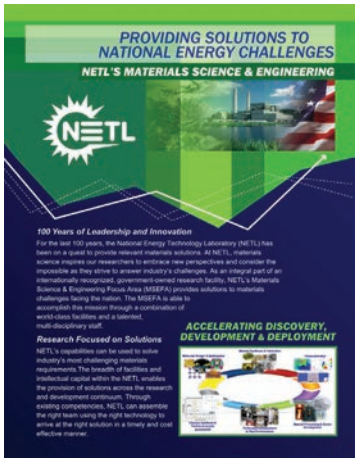
Strategic Fact Sheets and Brochures: NETL-RUA informational materials such as fact sheets and brochures are distributed to members of academic and industry communities at conferences and meetings. These brochures are designed to provide pertinent information about key capabilities and initiatives to cultivate new partnerships for innovation.

For example, in FY12, new fact sheets were developed for specific NETL-RUA initiatives (such as SGAs, SBEUC, and EDX). These communications products will be used to help cultivate new research partnerships for these initiatives.

An NETL Materials Science and Engineering brochure was created to promote the capabilities of NETL-RUA's cross-cutting expertise in the area of materials research and engineering.

This brochure highlights the history of NETL's materials research, its collaborative partnerships within academia and industry, technological advancements made by NETL-RUA members, and the world-class capabilities available to researchers.

The brochure can be viewed on the NETL website at http://netl.doe.gov/rua/about/AdvancedMaterialsBrochure.pdf



NETL Materials Science and Engineering Brochure

News Releases: NETL-RUA research efforts resulted in the distribution of 12 Techlines (NETL's version of a press release) describing innovations ranging from patent licensing of CO_2 removal sorbents to the installation of one of the world's fastest supercomputers at NETL. These Techlines created more visibility for the Alliance by increasing name recognition, improving the public's awareness of technological advances and achievements, and further promoting the Alliance's mission.

NETL-RUA Members Selected as Ambassadors in Science Pilot Program: In 2012, the NAS and the National Academy of Engineering (NAE) named Pittsburgh, PA, as the site for their Science & Engineering Ambassador Program.

The focus of this pilot program is *energy*, making Pittsburgh an obvious choice as it has become a nexus for coal, natural gas, nuclear, solar, and wind power

NETL-RUA Members NAE Ambassadors in Science

industries and research. Pittsburgh is also home to an impressive number of eminent scientists and engineers working on energy issues at some of the nation's top universities.

The goal of the program is to raise awareness about energy issues and help community members such as teachers, business leaders, and local media groups become comfortable with discussing energy issues with the community. The ambassadors are established, well-respected experts who come from academia, industry, or government; several Pittsburgh scientists and engineers have been selected as ambassadors to promote this goal.

In fact, a majority of the ambassadors are NETL-RUA members, including Jay Apt, Neil Donahue, and Edward S. Rubin from CMU; Brian Gleeson and Gregory Reed from Pitt; Christina Gabriel, President of the University Energy Partnership and a member of the NETL-RUA EC; and Brian Strazisar, Bryan Morreale, Alexandra Hakala, and Paul Ohodnicki of NETL.

The long-term goal of the Ambassador Program is to develop a replicable model that can be implemented in cities nationwide, building stronger relationships between scientists/engineers and their communities while improving citizens' engagement with current issues in science, technology, and medicine.

These NETL-RUA members will use this opportunity to educate the public about energy and raise awareness and visibility of the good work being done by NETL and its partners.

Media Outreach

NETL-RUA Technology Innovation Featured in Trade Publications: NETL-RUA research impacts a variety of technologies and has been featured in a number of trade journals and magazines.

Photonics Spectra Magazine

Prior NETL-RUA research on a laser spark plug was featured in the September 2012 issue of the trade magazine, *Photonics Spectra* (circulation 95,000).

This story entitled, "Laser Car Ignition Dream Sparks Multiple Approaches," by Laura Marshall, highlights the laser spark plug technology developed at NETL by Steven Woodruff and Dustin McIntyre. The article reviews the application of laser spark plugs to automobiles and draws heavily on the natural gas-fueled engine studies done at NETL.

The NETL-RUA has been recognized by various regional media outlets as a resource for energy innovation. The Pittsburgh Business Times featured an article on October 19, 2012, entitled "NETL, Universities Make Great Team." The article recognized the significant contributions of academic and industrial entities throughout the region to the energy sector and the up-and-coming technologies emerging from them.

The prominent research and educational resources provided by NETL-RUA are highlighted in the article as an example of the potential for economic growth in the region through its many research and commercialization opportunities. The

article anticipates significant international recognition of this energy sector growth due to the ongoing efforts of the NETL-RUA and its members.

NETL-RUA Cutting-Edge Research Results Shared with the Technical Community: A key output of NETL-RUA is the multitude of research reports, presentations, posters, and speeches that serve to disseminate the results of cutting-edge research stemming from NETL-RUA collaborative efforts.

Publication counts can be viewed as a measure of research productivity. In FY12, NETL-RUA published 159 peer reviewed papers (Appendix B), most of them jointly authored, describing work performed under the auspices of NETL-RUA research teams. This represents the baseline efforts of the researchers to publish in nationally and internationally recognized scientific and engineering journals. In addition, numerous ancillary contributions were made throughout the year by researchers as they provided poster presentations and reported results at technical conferences.

NETL-RUA community reach extends beyond the above mentioned totals as investigators contributed articles about their energy research in peer reviewed journals, which were not directly sponsored through NETL, but coincided with the mission and vision of the NETL-RUA.

The work generated and published by the NETL-RUA this past year provides an excellent foundation for future work and an expectation for greater success in 2013.

Internal Communication

NETL-RUA Spring Meeting: NETL-RUA members met at the Waterfront Place Hotel in Morgantown, West Virginia on March 9, 2012, for the Alliance's second annual spring meeting. Over 200 members, (including 31 by webcast) convened to greet friends and colleagues and learn about NETL-RUA progress and key initiatives.

Following a welcome from WVU provost Michele Wheatly, ORD Director Cindy Powell delivered the main address, which was followed by presentations on three NETL-RUA research initiatives. NETL-RUA Manager Juli Klara presented on R&D growth pathways, which was followed by presentations on the three current SGAs—Shale Gas, Grid Technology, and Rare Earths. Alliance research teams provided attendees with the opportunity to learn more about the work being accomplished and to develop future plans for research and growth, while Charter Committees met with "long-distance" members.

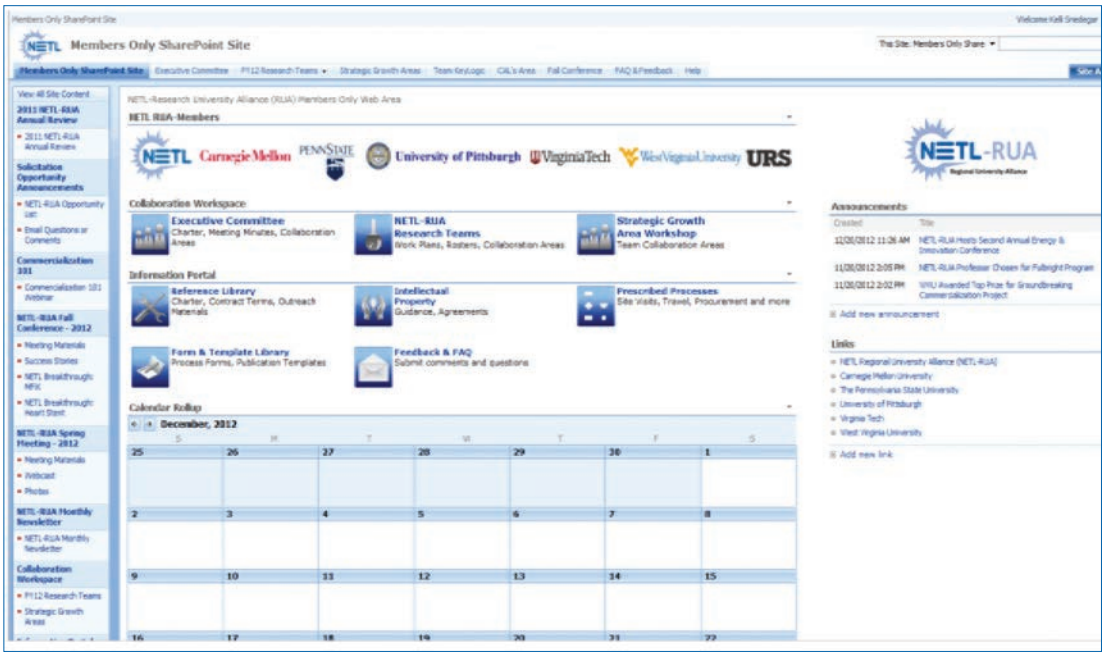
At the event, NETL Director Anthony Cugini acknowledged the Alliance's quick growth in just a few years, during which "we brought together five major universities, a very multifaceted government organization, and a major company to channel efforts and focus on a singular goal of building a regional powerhouse that could do fantastic and cutting-edge research."

Links to conference presentations and webcasts are available for viewing at http://www.netl.doe.gov/rua/events_archive.html on the NETL-RUA website.

NETL-RUA Members Only SharePoint Site (MOSS): This site, available to all NETL-RUA members, serves both as an information portal and workspace for teams and committees to share documents and collaborate. NETL-RUA research teams are given access to MOSS to provide them with a collaborative work environment with controlled access.

New to the site this year is a comprehensive list of prospects that Alliance members can use to quickly identify collaborative funding opportunities.

NETL-RUA Spring Meeting Presenters and Attendees



NETL-RUA MOSS

NETL-RUA eNews Newsletter: This monthly newsletter, distributed electronically to all NETL-RUA members, serves as a source of the latest information about NETL-RUA's research activities, as well as other important news. NETL-RUA eNews Newsletters are also available for viewing at http://www.netl.doe.gov/rua/events.html

NETL-RUA eNews Newsletter

Recognition

Awards

Council for Chemical Research (CCR) Honors NETL Collaborative Research: The CCR recognized Dave Berry, Daniel Haynes and Dushyant Shekwat (NETL); Mark Smith (URS); and Jerry Spivey (LSU) with a 2012 Research Collaboration Award for their work to develop novel pyrochlore catalysts for reforming of hydrocarbon fuels.

This award, given each year by CCR, honors a team of professionals in the field whose combined efforts have made an outstanding contribution to the advancement of chemistry-related science or engineering. CCR is a nonprofit organization dedicated to advancing research in chemistry, chemical engineering, and related disciplines.

Representing a collaboration of industry, academia, and other government agencies, the award-winning team demonstrated the superior function and value of the pyrochlore-based reforming catalyst, and has made significant advances in development and deployment of a commercially viable product.

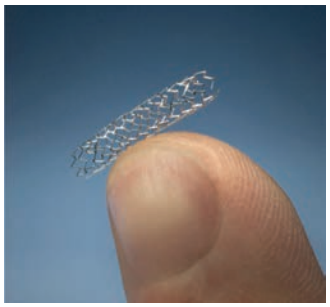
Developing stable catalysts for use in fuel reforming to produce hydrogen-rich synthesis gas is critical for enabling SOFC-based auxiliary power units (APUs) that can eventually be used in commercial power plants and commercialized on a wide-scale. The potential of this technology has recently been recognized through the execution of an exclusive licensing agreement with the Pyrochem Catalyst Corporation (PCC). NETL will continue to collaborate with PCC to further develop pyrochlore catalysts for use in fuel cell-based APUs and other commercial and military power applications.

NETL's Coronary Stents Team Earns DOE Secretary of Energy Achievement Award and Federal Laboratory Consortium (FLC) National Award (Excellence in Technology Transfer): Paul Turner and Paul Jablonski of NETL and Ed Argetsinger of URS earned two awards in 2012: a Secretary of Energy Achievement Award and an Excellence in Technology Transfer Award for their work in formulating a unique platinum-chromium alloy used for new-generation coronary stents. These awards add to the R&D 100 award they received in FY11 for this technology.

Coronary stents save lives by permitting blocked or restricted arteries to be reopened, allowing blood and oxygen to flow freely again to cardiac tissue. Coronary artery disease, or heart disease, is the leading cause of death in the United States, affecting more than 13 million Americans.

The stents, jointly developed by NETL and Boston Scientific Corporation Inc. (BSCI), are superior to older models and allow for treatment of such a broad range of patients, that they have captured nearly half of the U.S. and one-third of the international market, with sales of more than $4 billion.

The stents are made of a novel platinum chromium alloy, which makes it easier for doctors to see them on an x-ray and when inserting them in patients. The strength of the alloy makes the stent less likely to constrict once it is placed in a patient leading to lower rates of blood clotting. Finally, the new stent's relative thinness makes it easier to thread through or safely place in the difficult to navigate areas where an artery bends.



Small coronary stents made with a unique platinum-chromium alloy developed by NETL and Boston Scientific can open blocked arteries and save lives.

This alloy has recently been approved in Europe for use in peripheral stents—those used to repair damaged blood vessels in extremities (legs and arms)—and it is expected that these same stents will be approved for marketing in the United States within the next few months.

Results from this partnership also include the creation of 300 new jobs at BSCI alone, many of them in skilled, high paying engineering and production positions. More BSCI job creation is anticipated as new stent series are approved for marketing in the United States and the rest of the world.

In addition, well over 100 American workers are employed in the supply chain that produces these stents—exclusively in the United States—and ships them globally.

The Secretary's Awards, given annually, represent the highest level of internal non-monetary recognition for DOE employees.

The FLC Awards Program annually recognizes federal laboratories and their industry partners for outstanding technology transfer efforts. These awards have become one of the most prestigious honors in technology transfer.

For more information about the stent or these awards: http://www.netl.doe.gov/publications/press/2012/120508_stent_technology.html

AVESTAR System Wins Award: The FLC recognized Stephen Zitney (NETL), along with research engineers Eric Liese (NETL) and Priyadarshi Mahapatra (URS), with an Excellence in Technology Transfer Award for their work developing the AVESTAR™ system.

This world class AVESTAR Center at NETL is dedicated to accelerating progress toward achieving operational excellence for commercial-scale, clean energy plants. The AVESTAR dynamic simulator—a high-fidelity, real-time operator training system—provides initial hands-on training for operations, control, and safety of IGCC power plants and CO_2 capture systems.

By providing risk-free instruction outside of a working power plant, the AVESTAR system can help develop a qualified workforce that is well prepared to operate,

control, and manage advanced commercial-scale IGCC power plants with carbon capture that are predicted by experts to represent the future of clean coal technology.

IGCC systems offer many advantages over traditional plants, including cleaner operation, increased efficiency, and lower cost of electricity when capturing CO_2; they can also produce specialty chemicals, clean hydrogen, and transportation fuels. NETL partner, Fossil Consulting Services, provides a portfolio of 5- and 10-day courses at two AVESTAR centers at NETL and WVU in Morgantown, WV. The course offerings include both familiarization classes and comprehensive courses that instruct on background and theory, both followed by hands-on simulator sessions to put information learned into practice.

NETL and its partners are continuing to build the AVESTAR portfolio of dynamic simulators, 3-D virtual immersive training systems, and advanced research capabilities to satisfy industry's growing need for training and experience in the operation and control of clean energy plants. Future dynamic simulators under development include natural gas combined cycle and supercritical pulverized coal plants with post-combustion CO_2 capture.

NETL's FLC Technology Transfer Award recipients, Priyadarshi Mahapatra, Stephen Zitney, and Eric Liese

NETL Researcher Wins Hispanic Engineer National Achievement Awards Corporation (HENAAC) Award: Alexandra Hakala (NETL) has been honored with a Great Minds in STEM™ HENAAC award for Outstanding Technical Achievement.

Hakala's innovative and inspirational qualities and drive are just a few of the reasons she was chosen for this award. According to NETL Director Anthony Cugini, in just three years as a research scientist at NETL, "Dr. Hakala has emerged as a talented scientist, gifted leader, and an articulate ambassador for the Laboratory's research, its programs, and the importance of our work to the energy sector of the United States."

Hakala serves as the technical coordinator for shale gas research, managing multiple projects within NETL's ORD.

Alexandra Hakala in the laboratory at NETL

She leads two research teams in addition to performing her own research. One of these teams is developing knowledge that could lead to computational models for predicting risks associated with shale gas development. This research could increase confidence that processes used to tap the United States' abundant gas shale reservoirs are environmentally safe.

The second team is studying reactions that may occur along fractured pathways in a geothermal reservoir and developing detailed models of physical changes expected in unique geothermal systems.

In her free time, Hakala communicates her research to a wide audience through her published papers and national and international conference presentations, making a significant contribution to ongoing conversations on energy research. She also guides young scientists as they pursue graduate and post-graduate degrees, devoting time to her interns to ensure that they complete their thesis and lab work and have someone to depend on for career advice.

Great Minds in STEM considers nominees for their awards to be "top role models" in science, technology, engineering, and math (STEM) fields and uses the HENAAC

awards to "promote and highlight Hispanic engineers and scientists." These awards spotlight rising stars in STEM to encourage the next generation to pursue careers in these fields and motivate current STEM innovators to continue to connect with their Hispanic heritage.

NETL Funded Researcher Honored with a Presidential Early Career Award for Scientists and Engineers (PECASE): U.S. President Barack Obama named John Kitchin (CMU) as a recipient of a PECASE for his research on electrochemical separations for energy applications, which has the potential to enable clean coal technologies that meet DOE goals for carbon capture. Kitchin was also recognized for his dedication to educating the next generation of scientific leaders.

PECASE awards are the highest honor bestowed by the U.S. government on outstanding scientists and engineers who are early in their independent research careers.

Kitchin has made significant contributions to the development of carbon capture technology in his collaborations with NETL, advancing efforts to enable the environmentally responsible use of fossil fuels for electricity generation.

He was the first to demonstrate the use of an alkaline ion exchange membrane in the electrochemical separation of oxygen from air, which has the potential to displace cryogenic air distillation as the method for producing oxygen for oxy-combustion power generation. This advance also allows the use of inexpensive base-metal catalysts, and is closely linked to Kitchin's contributions to fundamental advances in the computational modeling and design of new catalyst materials, for which he received a research grant under DOE's 2010 Early Career Research Program.

Aside from his research and active support of NETL-RUA's carbon capture research team, Kitchen is an innovative teacher, having mentored 14 undergraduates and developed an interactive webinar series of lectures that were delivered live to grade school students. In appreciation of his dedication, he was awarded the Kun Li Teaching Award in 2010 for best lecturer in his department, as voted on by the senior class at CMU.

NETL-RUA Researchers Earn Prestigious Ceramic Industry Award for Published Work: In recognition of the valuable contribution of their published work to the ceramic industry, Jinichiro Nakano (URS); Kyei-Sing Kwong and James Bennett (NETL); Thomas Lam, formerly a Ph.D. student working at NETL; Laura Fernandez and Piyamanee Komolwit (CMU); and Professor Sridhar Seetharaman (CMU) earned the American Ceramic Society's prestigious 2012 Richard and Patricia Spriggs Phase Equilibria Award.

Deputy Secretary of Energy Daniel B. Poneman, John Kitchin, and NETL Laboratory Director Anthony Cugini

The American Ceramic Society recognized the team for its publication "Phase Equilibria in Synthetic Coal—Petcoke Slags (Al_2O_3-CaO-FeO-SiO_2-V_2O_3) under Simulated Gasification Conditions." The publication appears in *Energy and Fuels* 2011, 25, 3298-3306.

This research effort provided important information for understanding how to optimize materials performance in fuel-flexible gasifier systems, and was also recognized earlier this year with the Gustav-Eirich Award.

The American Ceramic Society presents this annual award to the author or authors of a published work that makes a valuable contribution to the field of phase-stability relationships in ceramic-based systems.

NETL-Developed Carbon Capture Technology Wins 2012 R&D 100 Award: NETL was recognized as a leader in the development of solid sorbent technology when it was awarded an R&D 100 Award for one of its solid sorbents. R&D 100 awards, known as the "Oscars of Invention," are selected by an independent panel of judges and the editors of *R&D Magazine*.

The award recognized the BIAS process, encompassing a portfolio of patented and patent-pending technologies for the capture of CO_2 from flue gas streams so that it can be used or stored to help control CO_2 emissions from power plants. The process encompasses a portfolio of techniques for the production of regenerable immobilized amine-based sorbents and provides a methodology for the capture of CO_2 from flue gas streams. Low-cost, regenerable amine-based sorbents offer many advantages over existing technologies, including increased CO_2 capture capacity, reduced corrosion, lower energy requirements and costs, and minimal water usage.

Amine-based sorbents are also scalable for use in industrial applications, including coal combustion and gasification-based power generating systems.

Application of this technology is expected to reduce the cost and energy use associated with more conventional scrubbing processes. The process can be used as a retrofit to older power plants that currently burn coal or applied to new, more efficient pulverized coal-fired power plants. Or it can capture CO_2 from utilities that combust oil or natural gas. BIAS sorbents are also being considered for other applications such as natural gas cleanup, life support systems/confined spaces, and air capture systems.

Led by McMahan (Mac) Gray of NETL, a team of NETL-RUA researchers including James Hoffman, Henry Pennline, Kenneth Champagne, Dan Fauth, and Yee Soong of NETL and Kevin Resnik of URS, worked to develop this process.

McMahan Gray conducts CO_2 sorbent testing in NETL's lab-scale sorbent test laboratory.

Additionally, team members Jessica Sosenko of NETL and Kathryn Klos of URS worked closely with strategic partner ADA-ES to license the BIAS process and to provide a mechanism for further R&D through a Cooperative Research And Development Agreement (CRADA) related to sorbent development. ADA-ES develops and commercializes innovative technologies to sustain the viability of coal as a critical national resource. Continued research under the CRADA has been successful and will continue until the beginning of 2013.

NETL-RUA Researchers Selected for Several Federal Executive Board (FEB) Awards: The Pittsburgh FEB has selected the following personnel from NETL for the following Excellence in Government Awards: Paul Ohodnicki, Jr. for Rookie of the Year, Gold Award; Robert Warzinski for Outstanding Professional Employee (Med/Scientific Field), Bronze Award; Steve Woodruff, Michael Buric, and Benjamin Chorpening of the Raman Sensor Team, Bronze Award; and Benjamin Chorpening and David Huckaby for the Community Service Award, Bronze Award.

Paul Ohodnicki, Rookie of the Year, is a materials scientist in the Chemistry and Surface Science Division working on high-temperature sensor materials for utility-scale power plant applications. He also interacts closely with groups working on catalysts, photocatalysts, and SOFCs by providing electron microscopy and technical support.

Robert Warzinski, Outstanding Professional Employee, is a leading researcher on CO_2 hydrates (formation) and works in the High Pressure Water Tunnel Laboratory located at NETL.

The Raman Sensor team earned a Bronze Award for developing a gas sensor for fuels which can give a full composition analysis in one second or less. Steve Woodruff, Ben Chorpening, and Michael Buric work on laser applications at NETL for diagnostics in combustion and optical sensors for combustion and bioengineering. Ben Chorpening and David Huckaby, whose research focuses on CFDs simulations, earned their Bronze Community Service Award for volunteer work with the Monongalia Youth Soccer Association, which runs recreational soccer in the spring and fall for about 1200 youth in Monongalia County, West Virginia.

Prestigious Title

Larry Banta
2012 Fulbright Program Scholar

NETL-RUA Principal Investigator and Professor Chosen for the Fulbright Scholar Program—WVU engineering professor and NETL-RUA PI Larry Banta has been chosen for the Fulbright Scholar Program sponsored by the Bureau of Educational and Cultural Affairs, U.S. Department of State. The Fulbright Scholar Program is a highly prestigious international award designed to increase mutual understanding between the people of the United States and those of other countries.

Banta was invited to the University of Genoa (UNIGE) in Italy to work on advanced energy generation and management. During his visit to UNIGE, he will be conducting research on several aspects of fuel cell and gas turbine hybrid electric generation and is looking forward to strengthening existing ties between UNIGE, NETL, and WVU. Banta's expertise in fuel cells significantly contributed to the research efforts and strategic goals of the NETL-RUA's Fuel Cells research team.

What to Expect in 2013

NETL-RUA will continue to build upon its record of accomplishments to strengthen its outreach and impact. This will be achieved by performing world-class research based on combined experimental and computational approaches, enhancing educational collaboration, accelerating commercialization of energy innovations, and expanding the breadth of NETL-RUA R&D.

NETL-RUA recipients (pictured) of the 2011 Mickey Leland Energy Fellowship working with an NETL-RUA researcher at NETL.

Enhancing Resources for Collaboration and Education

In FY13, NETL-RUA will provide additional capabilities to track FOAs, permit real-time collaboration to develop joint responses to funding prospects, and monitor proposals and new projects that leverage NETL-RUA funding.

NETL-RUA will continue to focus on educational initiatives in FY13. The launch of a new undergraduate intern program to encourage students to pursue advanced degrees in research and the award of travel grants to outstanding NETL-RUA research projects specifically to facilitate graduate student presentation of research results are at the forefront of these efforts.

Attendees networking at the second Annual E&I Conference held November 28–29, 2012, in Canonsburg, Pennsylvania.The conference brought together business and industry leaders from Pennsylvania, West Virginia, Ohio, and Virginia, as well as NETL-RUA members.

Moving Energy Innovations to the Marketplace

The Alliance will host, in collaboration with Catalyst Connection, a Third Annual E&I Conference in September 2013 to engage the region's energy researchers and manufacturing sector for advancement of innovations from laboratory to commercial application.

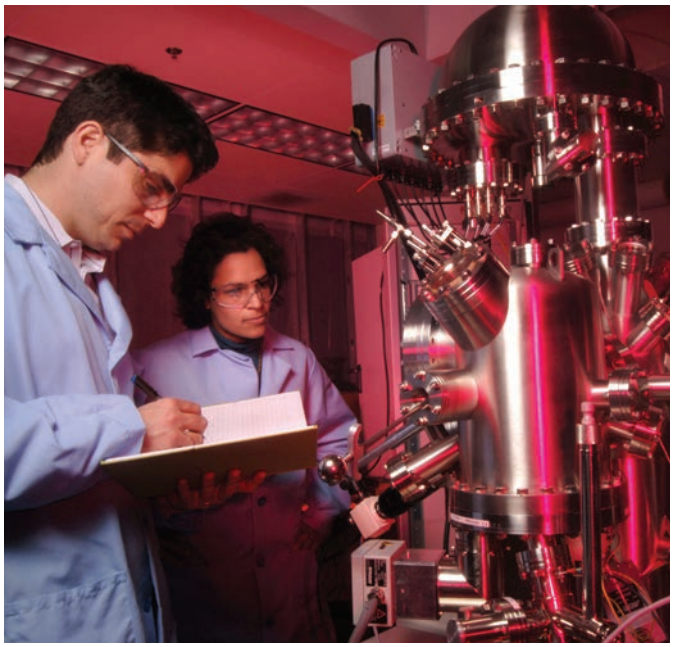
Implementing Strategies for Growth to Strengthen Outreach and Impact

FY13 will see continued emphasis on a growth strategy initiated by the EC. The two-pronged strategy emphasizes expanding NETL-RUA's portfolio by growing core FE research and expanding other related and high-potential research areas.

The SGAs, in their second year of existence, will work toward obtaining sustainable funding from industry partners and through establishment of joint research consortiums. For these opportunities, NETL-RUA will capitalize on its established industrial partnerships and concentrate on those industry sectors that, based on recent market analyses, have been identified as having technology needs that can be addressed by NETL-RUA expertise and capabilities. NETL-RUA will encourage new ideas by sponsoring an internal competition for research funding that recognizes existing outstanding research projects and soliciting new ideas from the broader university alliance population for innovative research concepts that further NETL's mission.

Finally, NETL-RUA will investigate strategies to integrate university energy-related initiatives with NETL's applied energy research expertise and the region's rich energy industry and entrepreneurial spirit to build technologies that provide a bridge to a sustainable energy future. NETL-RUA can have a greater impact on new products, processes, and jobs by capitalizing on regional partnerships.

Though much has been accomplished since the NETL-RUA was established, there is still much work to be done. The NETL-RUA will build on this momentum in FY2013 to sustain and accelerate progress.



Christopher Matranga (left) a researcher in the ORD at the DOE NETL, and Neetha Khan, a research scientist at NETL, prepare an experiment in NETL's Omicron Analysis and Surface Imaging System (OASIS). The OASIS system allows researchers to image individual atoms and determine the elemental composition of the first few atomic layers of surfaces relevant to FE applications.

Appendix A: FY2012 NETL-RUA Research Teams and Personnel

ADVANCED COMBUSTION

NETL Federal Project Manager: Randy Gemmen

NETL Team Technical Coordinator: Jeff Hawk

Name	Affiliation	Title
Gemmen, Randall	NETL	Division Director (DD)
Hawk, Jeffrey	NETL	Materials Research Engineer
Holcomb, Gordon	NETL	Materials Research Engineer
Jablonski, Paul	NETL	Metallurgist
Robey, Edward	URS	Contractor Project Lead
Argetsinger, Edward	URS	Engineering Technician
Burkey, Edward	URS	Engineering Technician

Name	Affiliation	Role	University Project Title
Seetharaman, Sridhar Zhu, Jingxi	CMU	PI Grad Student	Fundamental Examination of Deposit Compositions Associated with Fireside Corrosion
Meier, Gerald Yanar, Nazik Lutz, Michael	Pitt	PI Co-PI Grad Student	Fundamental Examination of Deposit Compositions Associated with Fireside Corrosion

ADVANCED GASIFICATION

NETL Federal Project Manager: Randy Gemmen

NETL Team Technical Coordinator: James Bennett

Name	Affiliation	Title
Baltrus, John	NETL	Research Chemist
Bennett, James	NETL	General Engineer (Leader)
Benyahia, Sofiane	NETL	General Engineer
Boyd, David	NETL	Engineering Technician
Breault, Ron	NETL	General Engineer
Carney, Janine	NETL	General Engineer
Chinn, Richard	NETL	Materials Research Engineer
Collins, Westley	NETL	Metallurgist
Curtis, Edward	NETL	Electronics Engineer
Danielson, Paul	NETL	Physical Science Tech
Gibson, LaTosha	NETL	General Engineer
Granite, Evan	NETL	Chemical Engineer
Hedges, Sheila	NETL	Research Chemist
Jordan Jr, Terry	NETL	Computer Engineer
Krabbe, Eric	NETL	Mechanical Engineer
Kwong, Kyei-Sing	NETL	Materials Research Engineer
Liese, Eric	NETL	Mechanical Engineer
Massoudi, Mehrdad	NETL	Mechanical Engineer
Mei, Joseph	NETL	Mechanical Engineer
Morreale, Bryan	NETL	General Engineer
Shadle, Lawrence	NETL	Physical Scientist
Shaffer, Franklin	NETL	General Engineer
Shahnam, Mehrdad	NETL	General Engineer
Siefert, Nicholas	NETL	Mechanical Engineer
Thomas, Hugh	NETL	Materials Research Engineer
Van Essendelft, Dirk	NETL	General Engineer
Vanosdol, John	NETL	Mechanical Engineer
Wang, Ping	NETL	General Engineer
Weber, Justin	NETL	General Engineer
Williamson, Kenneth	NETL	Computer Scientist
Yue, Paul Check	NETL	Physicist
Zitney, Stephen	NETL	General Engineer
Bergen, Mike	URS	Contractor Project Lead
Garg, Rahul	URS	Research Engineer
Li, Tingwen	URS	Research Engineer
Mahapatra, Priyadarshi	URS	Research Engineer
Means, Nicholas	URS	Research Engineer
Nakano, Jinichiro	URS	Research Scientist
Nicoletti, Philip	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Seetharaman, Sridhar	CMU	PI	Ash/Slag Management Testing, Analysis and Modeling CMU Support for Gasification Field Work Proposal (FWP)
Seetharaman, Sridhar Zhu, Jingxi	CMU	PI Post Doc	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Gellman, Andrew Miller, James	CMU	CAL PI	Warm Gas Clean-up In-Situ SEP Investigations of Palladium Interaction with Fuel Gas CMU Support for Gasification FWP
Pisupati, Sarma	PSU	PI	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Roy, Christopher	VT	PI	TRIG Model Development–UQ Quantification in Gasifier Simulations Numerical Uncertainty VT Support for Gasification FWP
Palacio, Diego Song, Xueyan	WVU	Grad Student PI	Ash/Slag Management, Analysis and Characterization WVU Support for Gasification FWP
Bhattacharyya, Debangsu Jones, Dustin Turton, Richard	WVU	Co-PI Grad Student PI	AVESTAR Center-Advanced Process Control WVU Support for Gasification FWP
Bhattacharyya, Debangsu Turton, Richard	WVU	PI Co-PI	AVESTAR Center-Aspen Dynamics Simulation and Load-Following Control of an IGCC Plant with CO_2 Capture WVU Support for Gasification FWP
Bhattacharyya, Debangsu Kasule, Job Turton, Richard	WVU	PI Grad Student PI	AVESTAR Center-Develop 1D Dynamic Model and ROM for Entrained-Flow Gasifier and RSC WVU Support for Gasification FWP
Chaudhari, Kiran Pandurang Turton, Richard Weiland, Nathan	WVU	Grad Student PI Co-PI	Low Rank Coal Optimization-Fundamental Gasification Code Development Soot Formation Kinetics/C3M WVU Support for Gasification FWP
Krishnaswamy, Ramalakshmi Kuhlman, John Michael	WVU	Grad Student PI	Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Weiland, Nathan	WVU	PI	RUA Support for Reducing Syngas Cooler Fouling and Unconverted Carbon Production
Bajura, Richard Dietiker, Jeff	WVU	CAL PI	TRIG Model Development Enhancement of Complex Geometry Representation capabilities in MFIX WVU Support for Gasification FWP
Bajura, Richard Musser, Jordan	WVU	PI PI	TRIG Model Development-Develop Co-feed TRIG Reduced Order Model WVU Support for Gasification FWP

CARBON CAPTURE

NETL Federal Project Manager: David Berry
NETL Team Technical Coordinator: David Luebke

Name	Affiliation	Title
Berry, David	NETL	DD
Duan, Yuhua	NETL	Physical Scientist
Fauth, Daniel	NETL	Research Chemist
Granite, Evan	NETL	Chemical Engineer
Gray, McMahan	NETL	Physical Scientist
Hoffman, James	NETL	Mechanical Engineer
Hopkinson, David	NETL	Mechanical Engineer
Jones, Kenneth	NETL	Research Chemist
Luebke, David	NETL	General Engineer
Matranga, Christopher	NETL	Research Chemist
Matuszewski, Michael	NETL	General Engineer
Morreale, Bryan	NETL	General Engineer
Myers, Christina	NETL	Chemical Engineer
Richards, George	NETL	Energy Sys Dynamics
Shadle, Lawrence	NETL	Physical Scientist
Siefert, Nicholas	NETL	Mechanical Engineer
Siriwardane, Ranjani	NETL	Physical Scientist
Steckel, Janice	NETL	Physical Scientist
Zandhuis, Paul	URS	Contractor Project Lead
Albenze, Erik	URS	Research Engineer
Culp, Jeffrey	URS	Research Scientist
Egbebi, Adefemi	URS	Research Scientist
Fisher, James	URS	Research Scientist
Hammache, Sonia	URS	Research Engineer
Hong, Lei	URS	Research Scientist
Kail, Brian	URS	Research Scientist
Lekse, Jonathan	URS	Research Engineer
Resnik, Kevin	URS	Research Engineer
Shi, Fan	URS	Research Scientist
Shi, Wei	URS	Research Scientist
Thompson, Robert	URS	Research Scientist
Wickramanayake, Wasala	URS	Research Engineer
Williams, Mark	URS	Research Director
Garg, Rahul	URS	Research Engineer
Li, Tingwen	URS	Research Engineer
Mahapatra, Priyadarshi	URS	Research Engineer
Means, Nicholas	URS	Research Engineer
Nakano, Jinichiro	URS	Research Scientist
Nicoletti, Philip	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Nulwala, Hunaid	CMU	PI	High Temperature Supported Ionic Liquid Membrane Synthesis - (CMS CRADA Funded Carbon Capture Support)
Kitchin, John	CMU	PI	Investigation and Mechanistic Study of Anime-Enriched Sorbents for Post-Combustion CO_2 Capture
Kitchin, John Alesi, Walter Demeter, Ethan Lee, Anita	CMU	PI Grad Student Grad Student Grad Student	Ion Exchange Resins as CO_2 Sorbents for Post-Combustion CO_2 Capture
Matyjaszewski, Krzysztof He, Hongkun	CMU	PI Grad Student	Synthesis and Characterization of Diblock Polymers with Nano-Scale Ordered Structures
Nulwala, Hunaid	CMU	PI	Synthesis of Ring-Complexing Ionic Liquids
Achary, Damodaran	Pitt	PI	Advanced NMR Characterization of Ionic Liquids
Enick, Robert	Pitt	PI	Development of High Molecular Weight PDMS
Jordan, Kenneth Rosi, Nathaniel Li, Tao	Pitt	PI Co-PI Grad Student	Development of Metal Organic Frameworks for Mixed Matrix Membranes for Post-Combustion CO_2 Capture
Jordan, Kenneth	Pitt	PI	Development of Polarizable Force Fields for Ionic Liquids
Johnson, Karl Zhang, Bo	Pitt	PI Grad Student	Molecular Modeling of Ionic Liquids for Post-Combustion CO_2 Capture Solvents
Achary, Damodaran	Pitt	PI	NMR Spectroscopic Studies of Ionic Liquids for CO_2 Capture and Separation
Janik, Michael Gao, Hongwei	PSU	PI Researcher	Computational Modeling of Novel Materials for Pre-Combustion CO_2 Removal
Lvov, Serguei Fedkin, Mark Beck, Justin	PSU	PI Co-PI Grad Student	Electrochemical In-Situ Monitoring of Metal Degradation in Carbon Sequestration Processes
Janik, Michael Gao, Hongwei	PSU	PI Researcher	High-Temperature CO_2 Separation from Gasifier Effluents
Li, Bingyun Jiang, Bingbing Noore, Jabeen	WVU	PI Post Doc Technician	Development of Phase Change Amino Acids for Use as Post-Combustion CO_2 Capture Solvents
Li, Bingyun Jiang, Bingbing Noore, Jabeen	WVU	PI Post Doc Technician	Hybrid Ionic Liquid Sorbents for Post-Combustion CO_2 Capture
Li, Bingyun Jiang, Bingbing Kish, Vincent Noore, Jabeen	WVU	PI Post Doc Technician Technician	Next Generation Materials for CO_2 Capture at WVU
Venna, Surendar Reddy	WVU	PI	Research Support for Pre-Combustion Membrane Ring-Complexing Supported Ionic Liquid Membranes
Bajura, Richard Marzouk, Osama	WVU	PI-CAL Co-PI	Task 4.0 Process Intensification, Module Design & Performance Assessment for H_2 Membrane FWP

CARBON STORAGE

NETL Federal Project Manager: Don Martello / Brian Strazisar

NETL Team Technical Coordinator: Brian Strazisar

Name	Affiliation	Title
Boyle, Edward	NETL	Research Chemist
Bromhal, Grant	NETL	General Engineer
Cardone, Carol	NETL	Physical Scientist
Clark III, John	NETL	Materials Research Engineer
Diehl, J Rodney	NETL	Physical Scientist
Dilmore, Robert	NETL	General Engineer
Edenborn, Harry	NETL	Research Microbiologist
Gerdemann, Stephen	NETL	Chemical Engineer
Goodman Hanson, Angela	NETL	Physical Scientist
Gulliver, Djuna	NETL	General Engineer
Hakala, Alexandra	NETL	Physical Scientist
Hammack, Richard	NETL	Physical Scientist
Hedges, Sheila	NETL	Research Chemist
Higgins, Glynn	NETL	Physical Science Tech
Howard, Bret	NETL	Research Chemist
Irdi, Gino	NETL	Physical Scientist
Karash, Andrew	NETL	General Engineer
Kutchko, Barbara	NETL	Physical Scientist
Lopano, Christina	NETL	Physical Scientist
Maurice, David	NETL	Materials Research Engineer
McIntyre, Dustin	NETL	Mechanical Engineer
McLendon, Thomas	NETL	General Engineer
Mroz, Thomas	NETL	Geologist
Pekney, Natalie	NETL	General Engineer
Romanov, Vyacheslav	NETL	Physical Scientist
Rose, Kelly	NETL	Geologist
Rosenbaum, Eilis	NETL	General Engineer
Sams III, James	NETL	Hydrologist
Schroeder, Karl	NETL	Physical Scientist
Seol, Yongkoo	NETL	Physical Scientist
Smith, David	NETL	Physical Science Tech
Soeder, Daniel	NETL	Physical Scientist
Soong, Yee	NETL	Chemical Engineer
Strazisar, Brian	NETL	Physical Scientist
Tran, Phuoc	NETL	Mechanical Engineer
Veloski, Garret	NETL	Research Chemist
Warzinski, Robert	NETL	Research Chemist
Wells, Arthur	NETL	Research Chemist
Ilconich, Jeff	URS	Contractor Project Lead
Anderson, Edward	URS	Engineer
Anderson, William	URS	Engineer
Briscoe, Jeffrey	URS	Electrical Supervisor
Bruner, Kathy	URS	Research Scientist

Name	Affiliation	Role	University Project Title
Karamalidis, Athanasios	CMU	PI	Arsenopyrite Precipitation and Dissolution Studies
Karamalidis, Athanasios	CMU	PI	Assessing the Potential Mobility of Organic Contaminants to Overlying Aquifers during Geologic Carbon Sequestration
Popova, Olga Small, Mitchell Thomas, Andrew	CMU	Grad Student PI Co-PI	Compare Methodologies by Applying to Site such as Illinois Basin or Oriskan
Popova, Olga Small, Mitchell Thomas, Andrew	CMU	Grad Student PI Co-PI	Evaluate Implications of Storage Estimates based on More Detailed Spatial Parameters using DOE Assessment Methodology
Gregory, Kelvin Lowry, Gregory	CMU	Co-PI PI	Impact of Microbial Mediated Precipitation on Flow and Seal Properties
Karamalidis, Athanasios	CMU	PI	International Interlaboratory Round Robin Study of Gas-Mineral-Fluid Interactions
Karamalidis, Athanasios Eseller, Kermal Gouguel, Christian	CMU	PI Post Doc Post Doc	On-Line Measurement of Ionic Species in Pressurized Cell by LIBS
Harbert, William	Pitt	PI	CO_2 Trapping Mechanisms in Clay Materials
Harbert, William	Pitt	PI	Effects of Pore-Filling Fluids on Seismic Wave Properties
Harbert, William	Pitt	PI	Field Data Analysis Determining the Location of CO_2 in the Reservoir
Jordan, Kenneth	Pitt	PI	Investigation of CO_2 Trapping Mechanisms in Clay Minerals
Stewart, Brian	Pitt	PI	Natural Isotope Tracers for Quantitative MVA (Stewart-Pitt)
Ertekin, Turgay	PSU	PI	Impact of Multiple Well Interferences and Brine Extraction on Pressure Limits
Westman, Erik	VT	PI	Double Difference Tomography to Detect Plum Locations Using Seismic Activity
Burbey, Thomas Zhou, Xue Jun	VT	PI Post Doc	Interpreting Mechanical Responses from a Reservoir to Determine Pressure Change
Yoon, Roe-Hoan	VT	PI	Role of Hydrophobic and Hydrophilic Mineral Surfaces on CO_2/Brine Flow through Pore-Scale Networks
Bodnar, Robert	VT	PI	Volumetric and Geochemical Effects Associated with Carbon Sequestration in Geologic Formations
Carr, Timothy Donaldson, Kurt Krammer, Chris McClain, Taylor Sharma, Maneesh	WVU	PI Co-PI Grad Student Grad Student Researcher	Primary Database Development and Primary Viewer Development
Mohaghegh, Shahab	WVU	PI	Reservoir Scale Impacts of Relative Permeabilities and Residual Saturations on Injectivity and Capillary Trapping
Mohaghegh, Shahab	WVU	PI	Sample Testing and Analysis Using Reservoir Models on Shales
Ameri, Samuel Aminian, Kashy	WVU	Co-PI PI	Sample Testing and Analysis Using the Precision Petrophysical Analysis Laboratory on Shales

CARBON STORAGE (cont.)

Name	Affiliation	Title
Carney, Casey	URS	Research Engineer
Crandall, Dustin	URS	Research Engineer
Damiano, Donald	URS	Industrial Hygienist
Disenhof, Corinne	URS	Research Scientist
Eastman, Harvey	URS	Research Scientist
Ference, Robert A	URS	Research Scientist
Garber, William	URS	Quality Sys Lead Engineer
Gill, Magdalena	URS	Research Intern
Haljasmaa, Igor	URS	Research Engineer
Harr, Bradley	URS	Process Engineer
Hill, Daniel	URS	Engineer
Jain, Jinesh	URS	Staff Scientist
Jarvis, Karl	URS	Engineering Technician
Juristy II, James	URS	Engineering Technician
Jursa, Christopher	URS	Research Scientist
King, Seth	URS	Research Scientist
Kuroski, James	URS	Engineering Technician
Lapeer, Roger	URS	Engineering Technician
Livengood, Kevin	URS	Engineering Technician
Martin, Donald	URS	Engineering Technician
Murin, Timothy	URS	Research Scientist
Myshakin, Eugene	URS	Research Scientist
Nielsen, Benjamin	URS	Research Engineer
Oberfoell, Jeffrey	URS	General Technician
Persichetti, Robert	URS	Mechanical Engineer
Roy, Robert	URS	Engineering Technician
Swenson, Dana	URS	Sr. Control System Engineer
Tennant, Bryan	URS	Engineering Technician
Tkach, John	URS	Engineering Technician
Wierzbicki, William	URS	Sr. Project Manager

CCSI

NETL Federal Project Manager: Cathy Summers

NETL Team Technical Coordinator: David Miller

Name	Affiliation	Title
Glier, Justin	NETL	ST (General Engineer)
Huckaby, E. David	NETL	Mechanical Engineer
Maurice, David	NETL	Materials Research Engineer
Miller, David	NETL	General Engineer
Shadle, Lawrence	NETL	Physical Scientist
Zitney, Stephen	NETL	General Engineer
Roger Cottrell	URS	Contractor Project Lead
Ma, Jinliang	URS	Research Engineer
Mahapatra, Priyadarshi	URS	Research Engineer
Montgomery, Christopher	URS	Consulting Engineer

Name	Affiliation	Role	University Project Title
Rubin, Edward	CMU	PI	Carbon CCSI Project Management (Task Set 0, Element 100)
Biegler, Lorenz Dowling, Alexander Grossmann, Ignacio Yang, Linlin Sahinidis, Nikolaos Cozad, Alison Yuan, Zhihong Siirola, Jeffrey	CMU	PI Grad Student PI Grad Student PI Grad Student Post Doc PI	Professional Services for Advanced Research (AR) Carbon CCSI in support of Element 3 – Process Synthesis and Design
Rubin, Edward	CMU	PI	Professional Services for Advanced Research (AR) CCSI in Support of the EC
Sahinidis, Nikolaos Vouzis, Panagiotis Yuan, Zhihong	CMU	PI Post Doc Post Doc	Professional Services for the CCSI Task 3 – Particle and Device Scale, Task Set 5 – Integration Framework, and Task Set 6 – Uncertainty Quantification
Gellman, Andrew Eslick, John	CMU	PI Post Doc	NETL CCSI Team – Element 3: Process Synthesis & Design
Bajura, Richard Saha, Kringan	WVU	CAL Co-PI	ARRA-Carbon CCSI Task Set 2 – Particle and Device Scale Models
Bhattacharyya, Debangsu Modekurti, Srinivasarao	WVU	PI Post Doc	CCSI
Mebane, David	WVU	PI	CCSI Team – Element 1 Basic Data and Models
Bhattacharyya, Debangsu Turton, Richard Paul, Prokash	WVU	PI Co-PI Grad Student	Sensor Placement Algorithm for at Least One Section in an IGCC Plant with CO_2 Capture

FUELS

NETL Federal Project Manager: Randy Gemmen

NETL Team Technical Coordinator: Dirk Link

Name	Affiliation	Title
Dogan, Omer	NETL	Materials Research Engineer
Haynes, Daniel	NETL	ST (Chem Engineer)
Howard, Bret	NETL	Research Chemist
Link, Dirk	NETL	Research Chemist
Morreale, Bryan	NETL	General Engineer
Poston, James	NETL	Physicist
Shekhawat, Dushyant	NETL	General Engineer
Smith, David	NETL	Physical Science Tech
Sorescu, Dan	NETL	Research Physicist
Ciocco, Mike	URS	Contractor Project Lead
Kail, Brian	URS	Research Scientist
Miller, Russell	URS	Research Specialist
Nielsen, Benjamin	URS	Research Engineer
Zandhuis, Paul	URS	Project Manager

Name	Affiliation	Role	University Project Title
Miller, James Kondratyuk, Petro	CMU	PI Co-PI	High-Performance, Poison-Tolerant Alloys for Hydrogen Separation Applications
Widom, Michael Huhn, William	CMU	PI Grad Student	Task 3.1.3 Material and Exposure Assessment
Gleeson, Brian	Pitt	PI	Protective-Scale Evolution and Stability in Complex Environments
Bajura, Richard Marzouk, Osama	WVU	PI Co-PI	Task 4.0 Process Intensification, Module Design & Performance Assessment for H2 Membrane FWP
Bajura, Richard Marzouk, Osama Belmaggio, Sharon Franks, Howard	WVU	PI Co-PI Technician Technician	Task 4.0 Module Design

FUEL CELLS

NETL Federal Project Manager: Randy Gemmen

NETL Team Technical Coordinator: Kirk Gerdes

Name	Affiliation	Title
Gerdes, Kirk	NETL	General Engineer
Mantz, Yves	NETL	Physical Scientist
Ohodnicki, Paul	NETL	General Engineer
Pineault, Richard	NETL	Research Chemist
Poston, James	NETL	Physicist
Shekhawat, Dushyant	NETL	General Engineer
Siefert, Nicholas	NETL	ST (Mechanical Engineer)
Kalapos, Thomas	URS	Contractor Project Lead
Ruehl, Dave	URS	Technician
Addis, Rick	URS	Technician

Name	Affiliation	Role	University Project Title
Salvador, Paul Picard, Yoosuf Neelam Bhattacharya, Sudip	CMU	PI Co-PI Post Doc	FIB-SEM Microstructure Reconstructions
Chen, Long-Qing	PSU	PI	Cathode Evolution by Coarsening
Celik, Ismail Pakalapati, Suryanarayana Raju	WVU	PI Co-PI	Dynamic 3D Multi-Physics Cathode/Anode Model
Liu, Xingbo Gong, Mingyang	WVU	PI Post Doc	Oxygen Reduction Reaction Model
Finklea, Harry Chen, Xioake Jony, Mahfuzur Rahman	WVU	PI Grad Student Grad Student	Cathode Cation Segregation
Song, Xueyan	WVU	PI	Cathode Intergranular Phase Growth Analysis
Song, Xueyan Chen, Yun	WVU	PI Post Doc	Anode Intergranular Phase Growth Analysis
Song, Xueyan	WVU	PI	Evaluation of Electrolyte Degradation
Sabolsky, Edward Gandavarapu, Sodith Kumar, Reddy	WVU	PI Researcher Researcher	Scale-up of Engineered Foam Cathode to SECA Scale
Song, Xueyan	WVU	PI	TEM Analysis of Industrial SOFC Stack Samples

ICMI

NETL Federal Project Manager: Cathy Summers

NETL Team Technical Coordinator: Ronald Breault/George Richards

Name	Affiliation	Title
Huckaby, David	NETL	Lead - Element 310
Straub, Douglas	NETL	Lead - Element 320, 330
Chorpening, Benjamin	NETL	Lead - Element 340
Siriwardane, Ranjani	NETL	Lead - Element 350
Summers, Cathy	NETL	Lead - Element 360
Dilmore, Robert	NETL	Lead - Element 410
Matranga, Christopher	NETL	DOE Lead - Element 420
Klara, Julianne	NETL	Lead - Element 520, 530
Carpenter, Stephen	URS	Project Coordinator - Lead 320, 360
Gallagher, Michael	URS	Lead - Element 310
Fisher, James	URS	Lead - Element 330
Charley, Jared	URS	Lead - Element 340
Miller, Duane	URS	Lead - Element 350
Siegel, Joel	URS	Lead - Element 410
Ciocco, Michael	URS	Lead - Element 420

Name	Affiliation	Role	University Project Title
Kitchin, John	CMU	PI	ICMI Support for Oxygen Carrier Interaction Studies
Greve, David	CMU	PI	Support for Solids Flow Measurement Sensor Development at High Temperature for CLC
Jin, Rongchao Kumar, Santosh	CMU	PI Grad Student	Atomically Precise Metal Nanoclusters for Catalytic CO_2 Utilization
Jordan, Kenneth Thakur, Anshuman	Pitt	PI Grad Student	Computational Support Sorbents and Catalysts of Photoactive Materials
Natesakhawat, Sittichai	Pitt	PI	Heterogeneous Catalysis of Photoactive Materials
Veser, Goetz	Pitt	PI	ICMI Support for Oxygen Carrier Interaction Studies
Ding, Mengning	Pitt	Grad Student	Oxygen Carrier Analytical Support
Blumsack, Seth Briggs, Ronald	PSU	PI Co-PI	Economic Assessment of CO_2 Storage in Shale
Ertekin, Turgay	PSU	PI	Numerical Modeling of CO_2 Injection into Depleted Shale Gas Reservoirs
Yoon, Roe-Hoan Cha, Jong-Ho	VT	PI-CAL Researcher	Evaluation of Hydrate Formation Processes for Treatment of High-Salinity ICS Produced Water
Lewis, James Wang, Hong Haycock , Barry Ranasingha, Oshadha Underwood, Mary	WVU	PI Researcher Post Doc Grad Student Grad Student	ARRA-Computational Support Sorbents and Catalysts of Photoactive Materials
Underwood, Mary	WVU	Grad Student	Novel ICMI
Mohaghegh, Shahab	WVU	PI	Numerical and Artificial Intelligence Modeling of CO_2 Injection into Depleted Shale Gas Reservoirs American Recovery and Reinvestment Act
Siriwardane, Hema	WVU	PI	Numerical Modeling of CO_2 Injection into Depleted Shale Gas Reservoirs
Aminian, Kashy Ameri, Samuel	WVU	PI Co-PI	Shale Gas Porosity, Permeability, Adsorption, and Effects of Net Stress under Representative Pressures using the WVU Precision Petrophysical Analysis Lab

IPT

NETL Federal Project Manager: Cathy Summers

NETL Team Technical Coordinator: David Alman

Name	Affiliation	Title
Alfonso, Dominic	NETL	Physical Scientist
Anderson, Richard	NETL	Research Chemist
Benyahia, Sofiane	NETL	General Engineer
Brown, Thomas	NETL	General Engineer
Buric, Michael	NETL	General Engineer
Carney, Janine	NETL	General Engineer
Casleton, Kent	NETL	Physical Scientist
Chorpening, Benjamin	NETL	Mechanical Engineer
Clark III, John	NETL	Materials Research Engineer
Duan, Yuhua	NETL	Physical Scientist
Ferguson, Donald	NETL	Mechanical Engineer
Gerdes, Kirk	NETL	General Engineer
Huckaby, David	NETL	Mechanical Engineer
Manivannan, Ayyakkannu	NETL	General Engineer
Maurice, David	NETL	Materials Research Engineer
Morreale, Bryan	NETL	General Engineer
Ochs, Thomas	NETL	General Engineer
Ohodnicki, Paul	NETL	General Engineer
Oryshchyn, Danylo	NETL	Mechanical Engineer
Shahnam, Mehrdad	NETL	General Engineer
Shekhawat, Dushyant	NETL	General Engineer
Sidwell, Todd	NETL	Mechanical Engineer
Sorescu, Dan	NETL	Research Physicist
Steckel, Janice	NETL	Physical Scientist
Strakey, Peter	NETL	Physical Scientist
Straub, Douglas	NETL	Mechanical Engineer
Tucker, David	NETL	Physical Scientist
Tucker, Mark	NETL	Engineering Technician
Wen, Youhai	NETL	Materials Research Engineer
Woodruff, Steven	NETL	Research Chemist
Woodside, Charles	NETL	General Engineer
Yip, M. Joseph	NETL	Mechanical Engineer
Wierzbicki, William	URS	Contractor Project Lead
Cottrell, Roger	URS	Contractor Project Manager
Anderson, Edward	URS	Engineering
Angeline, Gerald	URS	Engineering Technician
Carney, Casey	URS	Research Engineer
De Nyago, Tafen	URS	Research Scientist
Deng, Xingy	URS	Research Scientist
Gao, Michael	URS	Research Scientist
Harr, Bradley	URS	Process Engineer

Name	Affiliation	Role	University Project Title
Jaramillo, Paulina Apt, Jay Blanco, Christian	CMU	PI Co-PI Grad Student	Coal Power Plant Operations in a System with Increased Wind Power
Apt, Jay Jaramillo, Paulina Lueken, Roger	CMU	PI Co-PI Grad Student	Fossil Plan Mothball and Reactivation decisions with Increase Wind Power
Seetharaman, Sridhar	CMU	PI	Fundamental Examination of Deposit Compositions Associated with Fireside Corrosion
Rubin, Edward Kietzke, Karen Mantriprada, Hari Zhai, Haibo Glier, Justin Versteeg, Peter	CMU	PI Researcher Researcher Researcher Grad Student Grad Student	Integrated Environmental Control Model
Nulwala, Hunaid Cozad, Alison	CMU	PI Grad Student	Mg Battery Development
Greve, David	CMU	PI	Surface Acoustic Waves Sensor Development
Rubin, Edward Kietzke, Karen Mantriprada, Hari Zhai, Haibo Borgert, Kyle	CMU	PI Researcher Researcher Researcher Grad Student	The Role of Simulation and Modeling in Accelerating CO_2 Capture Technology
Hug, Gabriela McHenry, Michael DeGeorge, Vincent Zhu, Dinghuan	CMU	PI Co-PI Grad Student Grad Student	The Next Generation Power Converter: Smart Control Methodology
Meier, Gerald Yanar, Nazik	Pitt	PI Co-PI	Fundamental Examination of Deposit Compositions Associated with Fireside Corrosion
Givi, Peyman	Pitt	PI	LES of Sandia Half-Scaled Dump Combustor
Kumta, Prashant	Pitt	PI	Mg Battery Development
Star, Alex	Pitt	PI	Synthesis and Characterization of SiC Nanostructures for Sensors
Reed, Gregory	Pitt	PI	The Next Generation Power Converter: System Level Modeling
Liu, Zi-Kui Shang, Shun-Li	PSU	PI Co-PI	Computational and Experimental Investigations of Thermodynamic and Physical Properties of Complex Slags in Electro Slag Remelting (ESR)
Wang, Donghai	PSU	PI	Magnesium Battery Development
Haworth, Daniel	PSU	PI-CAL	PDF-Based Models for Oxy-Coal Combustion

IPT (cont.)

Name	Affiliation	Title
Hart, Chad	URS	Engineering Technician
Hill, Daniel	URS	Engineer
Kirby, Travis	URS	Research Engineer
Lee, Junseok	URS	Research Scientist
Montgomery, Christopher	URS	Consulting Engineer
Nelson, Janet	URS	Research Engineer
Persichetti, Robert	URS	Mechanical Engineer
Sears, John	URS	Research Engineer
Simonyi, Thomas	URS	Research Scientist
Thewlis, Tracy	URS	Mechanical Engineer

Name	Affiliation	Role	University Project Title
Santavicca, Domenic	PSU	PI	The Effect of EGR on the Performance and Operability of Lean Premixed Combustors
Dobbs, Greg Blumsack, Seth	PSU	PI Co-PI	The Next Generation Power Converter: Demonstration Site Plan & Development
Tafti, Danesh	VT	PI	Acceleration of MFIX
Tafti, Danesh	VT	PI	Heat and Mass Transfer in Porous Sorbent Particles
Vandsburger, Uri Shiver, Samuel	VT	PI Grad Student	Methods of Pulse Smoothing of Pressure Gain Combustion Events towards Enhanced Turbine Efficiency and Reliability
Murayama, Mitsu Monsegue, Niven Reynolds, William	VT	PI Co-PI Co-PI	Multi-scale Microstructure Analysis of High-Temperature Structural Materials
Ekkad, Srinath	VT	PI	Particle Stochastic Analysis with Minimal Sampling
Boroyevich, Dushan	VT	PI	The Next Generation Power Converter: Converter Topology
Weiland, Nathan Bedick, Clinton	WVU	PI Researcher	Fundamental Combustion Studies
Dietiker, Jeff Bajura, Richard	WVU	PI CAL	MFIX Acceleration
Celik, Ismail Escobar, Sergio Escobar-Vargas, Jose	WVU	PI Grad Student Grad Student	Simulation and Validation for Innovative Energy Concepts (S&V-IEC): WVU Combustion Modeling
Bhattacharyya, Debangsu Turton, Richard	WVU	PI Co-PI	Techno-Economic Optimization of Process and Energy Plants with Integrated CO_2 Capture and Utilization Processes
Bajura, Richard	WVU	PI	CFD Support of High-Temperature Oxy-Fuel Systems for Magnetohydrodynamics Applications
Banta, Larry	WVU	PI	Sensors and Advanced Controls Testing in Hyper – VE-Suite / HYPER Linkage
Famouri, Parviz Fallah, Yaser Khushalani-Solank, Sarika Nasirian, Neda Ramachandran, Roopa	WVU	PI Co-PI Co-PI Grad Student Grad Student	The Next Generation Power Converter: Interface & Communication Protocols
Liu, Zi-Kui Shang, Shun-Li	PSU	PI	Computational and Experimental Investigations of Thermodynamic and Physical Properties of Complex Slags in ESR

IPT (cont.)

Name	Affiliation	Role	University Project Title
Monsegue, Niven Murayama, Mitsu Reynolds, William	VT	Co-PI PI Co-PI	Multi-scale Microstructure Analysis of High-Temperature Structural Materials
Kumta, Prashant	Pitt	PI	Materials Science and Engineering, "Energy Storage – EERE Research Support"
Wu, Nianqiang Zhi, Mingjia	WVU	PI Post Doc	Nanomaterials for Energy Storage

NRAP

NETL Federal Project Manager: Cathy Summers

NETL Team Technical Coordinator: George Guthrie/Grant Bromhal

Name	Affiliation	Title
Boyle, Edward	NETL	Research Chemist
Bromhal, Grant	NETL	General Engineer
Clark III, John	NETL	Materials Research Engineer
Dilmore, Robert	NETL	General Engineer
Gerdemann, Stephen	NETL	Chemical Engineer
Goodman Hanson, Angela	NETL	Physical Scientist
Hakala, Alexandra	NETL	Physical Scientist
Hammack, Richard	NETL	Physical Scientist
Hedges, Sheila	NETL	Research Chemist
Higgins, Glynn	NETL	Physical Science Tech
Huerta, Nicolas	NETL	ST (Physical Science)
Irdi, Gino	NETL	Physical Scientist
Karash, Andrew	NETL	General Engineer
Kutchko, Barbara	NETL	Physical Scientist
Lacher Jr, Clement	NETL	Engineering Technician
Lopano, Christina	NETL	Physical Scientist
Maurice, David	NETL	Materials Research Engineer
McIntyre, Dustin	NETL	Mechanical Engineer
McLendon, Thomas	NETL	General Engineer
Mroz, Thomas	NETL	Geologist
Romanov, Vyacheslav	NETL	Physical Scientist
Rosenbaum, Eilis	NETL	General Engineer
Seol, Yongkoo	NETL	Physical Scientist
Smith, David	NETL	Physical Science Tech
Stanko, Dennis	NETL	Physical Science Tech
Strazisar, Brian	NETL	Physical Scientist
Verba, Circe	NETL	ST (Physical Scientist)
Warzinski ,Robert	NETL	Research Chemist
Webster, Daniel	NETL	Engineering Technician
Wells, Arthur	NETL	Research Chemist
Wells, Jimmy	NETL	Engineering Technician
Wells, Terrance	NETL	Engineering Technician
Wierzbicki, William	URS	Contractor Project Lead
Crandall, Dustin	URS	Research Engineer
Disenhof, Corrine	URS	Research Scientist
Ilconich, Jeffrey	URS	Project Support
King, Seth	URS	Research Scientist
Lindner, Ernest	URS	Research Engineer
Myshakin, Eugene	URS	Research Scientist
Sams, Neal	URS	Fellow R&D Scientist

Name	Affiliation	Role	University Project Title
Dzombak, David Zhang, Liwei	CMU	PI Grad Student	Acid Gas Interactions with Seal Materials under Geologic Sequestration Conditions
Karamalidis, Athanasios	CMU	PI	Conduct Site-Independent Generalized Studies Including Laboratory Experiments to Define the Impact of CO_2 Operations on the release of Contaminants and their Impact to Receptors
Small, Mitchell Nakles, David	CMU	PI PI	Development of an Integrated Risk Assessment Framework to Support Adaptive Site Management for Geologic CO_2 Sequestration
Small, Mitchel Karamalidis, Athanasios Wang, Zan	CMU	PI Co-PI Grad Student	Performance Evaluation and Integration of Multiple Deep Subsurface CO_2 Leak Detection Monitoring Technologies
Nakles, David Sahinidis, Nikolaos Zhang, Yan	CMU	Co-PI PI Grad Student	Risk Assessment in CO_2 Geologic Sequestration
William Harbert	Pitt	PI	Assess Remaining Key Science Gasp is Sequestration Risk Assessment
Brantley, Susan	PSU	PI	Assess Key Field Data Needs/Opportunities
Li, Li	PSU	PI	Development of a Reactive Transport Model for the Evolution of Fracture Properties under Conditions Relevant to CO_2 Sequestration
Karpyn, Zuleima Cao, Peilin	PSU	PI Grad Student	Experimental Investigation of Conditions Affecting Wellbore Integrity due to Chemical Reaction using X-ray micro CT imaging
Burgos, William	PSU	PI	Geo Chemical Transformations Caused by CO_2 Injection or Leakage
Li, Li Brunet, Jean-Patrick Leopold Heidari, Peyman	PSU	PI Researcher Grad Student	Multiphase Reactive Transport Processes Associated with Wellbore Cement Degradation during CO_2 Leakage
Wilson, Thomas	WVU	PI	Fault and Fracture Zone Detection and Reduced Order Fracture Model Development for Risk Assessment
Mohaghegh, Shahab	WVU	PI	Update Component Models for Calculating Risk Profiles
Siriwardane, Hema Gondle, Rajkumar	WVU	PI Post Doc	Use of Pressure and Displacement Signatures to Estimate Reservoir Storage Potential and Identify Possible Fault Activation in the Cap Rock During CO_2 Injection

TURBINES THERMAL MANAGEMENT

NETL Federal Project Manager: Randy Gemmen

NETL Team Technical Coordinator: Maryanne Alvin

Name	Affiliation	Title
Alvin, Maryanne	NETL	DD
Beer, Stephen	NETL	Physicist
Casleton, Kent	NETL	Physical Scientist
Gemmen, Randall	NETL	DD
Sidwell, Todd	NETL	Mechanical Engineer
Straub, Douglas	NETL	Mechanical Engineer
Tucker, Mark	NETL	Engineering Technician
Robey, Edward	URS	Contractor Project Lead
Riley, Jeffrey	URS	Engineering Technician

Name	Affiliation	Role	University Project Title
Gleeson, Brian	Pitt	PI-CAL	Diffusion Barrier Coatings (FWP 2012.03.02 - Advanced Energy Systems-Turbine Thermal Management Task 3.2)
Chyu, Minking Siw, Sean	Pitt	PI Grad Student	Internal and Transpiration Cooling (FWP 2012.03.02 - Advanced Energy Systems-Turbine Thermal Management Task 2.1)
Chyu, Minking Miller, Nicolas	Pitt	PI Grad Student	Trailing Edge Cooling (FWP 2012.03.02 - Advanced Energy Systems-Turbine Thermal Management Task 2.2)
Barringer, Michael Miller, James Thole, Karen	PSU	Co-PI Researcher PI	Rotating Rig Facility Development (FWP 2012.3.02 - Advanced Energy Systems-Turbine Thermal Management Task 5.1)
Ekkad, Srinath LeBlanc, Christopher Ramesh, S.	VT	PI Co-PI Co-PI	Film Cooling (FWP 2012.03.02 - Advanced Energy Systems-Turbine Thermal Management Task 2.3)

UDW AND FRONTIER REGIONS

NETL Federal Project Manager: Jamie Brown

NETL Team Technical Coordinator: Kelly Rose

Name	Affiliation	Title
Gamwo, Isaac	NETL	Chemical Engineer
Hawk, Jeffrey	NETL	Materials Research Engineer
Kutchko, Barbara	NETL	Research Scientist
Morreale, Bryan	NETL	General Engineer
Rose, Kelly	NETL	Research Scientist
Rosenbaum, Eilis	NETL	General Engineer
Strazisar, Brian	NETL	Physical Scientist
Warzinski, Robert	NETL	Research Chemist
Siegel, Joel	URS	Contractor Project Lead
Haljasmaa, Igor	URS	Physical Scientist
Disenhof, Corrine	URS	Research Scientist
Tapriyal, Deepak	URS	Research Engineer

Name	Affiliation	Role	University Project Title
Enick, Robert Baled, Hseen	Pitt	PI Grad Student	Quantifying Complex Fluid-phase Properties at High Pressure/High Temperature
Heasley, Keith Mishra, Brijes Zhang, Peng	WVU	PI Co-PI Grad Student	Advanced Rock Mechanics Testing of Rocks Under HTHP
Liu, Xingbo Collins, Greg Chen, Ting	WVU	PI Post Doc Grad Student	Experimental and Numerical Evaluation of Key Metal-Based Failures
Anderson, Brian Garapati, Nagasree	WVU	PI Grad Student	Numerical Simulation in Support of the Ignik Sikumi #1 Well and Associated Reservoirs
Anderson, Brian	WVU	PI	Plume Modeling for High-Pressure Water Tunnel Facility
Mohaghegh, Shahab	WVU	PI	Deepwater Horizon Litigation Response

UNCONVENTIONAL RESOURCES

NETL Federal Project Manager: Jamie Brown

NETL Team Technical Coordinator: Ale Hakala

Name	Affiliation	Title
Bromhal, Grant	NETL	General Engineer
Dilmore, Robert	NETL	General Engineer
Hakala, Alexandra	NETL	Research Scientist
Hammack, Richard	NETL	Research Scientist
Pekney, Natalie	NETL	Research Scientist
Rose, Kelly	NETL	Geologist
Sams III, James	NETL	Hydrologist
Schroeder, Karl	NETL	Research Scientist
Strasizar, Brian	NETL	Research Scientist
Veloski, Garret	NETL	Research Chemist
Murin, Tim	URS	Contractor Project Lead
Crandall, Dustin	URS	Research Engineer
Garber, William	URS	Quality Sys Lead Engineer
Jain, Jinesh	URS	Staff Scientist
Schuller, William	URS	Research Scientist
Siegel, Joel	URS	Project Support

Name	Affiliation	Role	University Project Title
Gregory, Kelvin	CMU	PI	Fate of Naturally Occurring Radioactive Material in Flowback and Produced Waters from Shale Gas Development Sites
Robinson, Allen	CMU	PI	Fugitive Air Emissions from Point Sources with Emphasis on Methane
Donahue, Neil Anirban, Roy	CMU	PI Grad Student	Secondary Photo-Oxidation of Diesel Emissions with Application at the Marcellus Shale Test Site
Enick, Robert	Pitt	PI	CO_2 Soluble Surfactants for Improved Mobility Control
Capo, Rosemary Macpherson, Gwendolyn	Pitt	PI Researcher	Evaluate Isotopic Compositions of Geologic End-Members and Fluid Samples
Vidic, Radisav	Pitt	Co-PI	Fate of Naturally Occurring Radioactive Material in Flowback and Produced Waters from Shale Gas Development Sites
Harbert, William Hur, Tae Bong	Pitt	PI Post Doc	Perform Baseline Geophysics and Modeling prior to Well Pad Construction and Drilling
Stewart, Brian Macpherson, Gwendolyn	Pitt	PI Researcher	Rapid Analysis Methods for Sr Isotopes with Multicollector ICP-MS Techniques
Bain, Daniel	Pitt	PI	Characterizing Salient Properties of Legacy Wells Located over the Marcellus Shale
McCawley, Michael	WVU	PI	Air and Environmental Sampling Around Marcellus Shale Gas Drilling Operations
Wood, Petra	WVU	PI	Baseline Environmental Characterization (Avian) Prior to Site Well-Pad Construction and Drilling
Hopkinson, Leslie Mack, Ben O'Neal, Melissa Streets, David	WVU	PI Co-PI Co-PI Grad Student	Impacts to Small Watersheds from Shale Development
Siriwardane, Hema	WVU	PI	Prediction of Fracture Propagation into Adjacent Reservoirs Using Field and Laboratory Data for Modeling Constraints
Sharma, Shikha Sack, Andrea	WVU	PI Grad Student	Stable Isotopes as Indicators of Fluid Sources and Fluid-Rock Interactions in Complex Geological Systems
Carr, Timothy	WVU	PI	Unconventional Resource Analysis Using Geographic Information Systems in Support for Shale Risk Assessment, and Evaluation of Methane Sources in Shallow Geologic Units in the Marcellus Shale Region

Appendix B: FY2012 NETL-RUA Peer-Reviewed Publications

Alesi, W. Richard, Jr.; Kitchin, John R. "Evaluation of a Primary Amine-Functionalized Ion-Exchange Resin for CO_2 Capture." *Industrial & Engineering Chemistry Research* 51, no.19 (May 2012): 6907–6915, DOI: 10.1021/ie300452c.

Alfonso, Dominic R. "Influence of Sulfur Poisoning on CO Adsorption on Pd(100)." *Topics in Catalysis* 55, no. 5-6 (June 2012): 267–279, DOI: 10.1007/s11244-012-9792-4.

Anderson, Karl; Bhatnagar, Gaurav; Crosby, Daniel; Hatton, Greg; Manfield, Philip; Kuzmicki, Adam; Fenwick, Nevi; Pontaza, Juan; Wicks, Moye; Socolofsky, Scott; Brady, Cole; Svedeman, Steve; Sum, Amadeu K.; Koh, Carolyn Levine, Jonathan; Warzinski, Robert P.; Shaffer, Franklin. "Hydrates in the Ocean beneath, around, and above Production Equipment." *Energy & Fuels* 26, no. 7 (July 2012):4167–4176, DOI: 10.1021/ef300261z.

Ayyalasomayajula, Krishna K.; Fang Yu-Yueh; Singh, Jagdish P.; McIntyre, Dustin L.; Jain, Jinesh. "Application of laser-induced breakdown spectroscopy for total carbon quantification in soil samples." *Applied Optics* 51, no.7 (March 2012):B149–B154.

Ayyalasomayajula, Krishna K.; McIntyre, Dustin L.; Jain, Jinesh; Singh, Jagdish P.; Fang Yu-Yueh. "Determination of elemental impurities in plastic calibration standards using laser-induced breakdown spectroscopy." *Applied Optics* 51, no. 7, (March2012): B143–B148.

Baled, Hseen; Enick, Robert M.; Wu, Yue; McHugh, Mark A.; Burgess, Ward; Tapriyal, Deepak; Morreale, Bryan D. "Prediction of hydrocarbon densities at extreme conditions using volume-translated SRK and PR equations of state fit to high temperature, high pressure PVT data." *Fluid Phase Equilibria* 317 (March 2012): 65–76, DOI: 10.1016/j.fluid.2011.12.027.

Beatty, William Lee; Schroeder, Karl; Beatty, Candace L. Kairies. "Mineralogical Associations of Mercury in FGD Products." *Energy & Fuels* 26, no. 6, (June 2012): 3399–3406, DOI: 10.1021/ef300033u.

Benyahia, Sofiane. "Analysis of Model Parameters Affecting the Pressure Profile in a Circulating Fluidized Bed." *AIChE Journal* 58, no. 2 (February 2012): 427–439, DOI: 10.1002/aic.12603.

Benyahia, Sofiane; Sundaresan, Sankaran. "Do we need sub-grid scale corrections for both continuum and discrete gas-particle flow models?" *Powder Technology* 220, Special Issue: SI, (April 2012):2–6, DOI: 10.1016/j.powtec.2011.10.052.

Bhavsar, Saurabh; Najera, Michelle; Veser, Goetz. "Chemical Looping Dry Reforming as Novel, Intensified Process for CO_2 Activation." *Chemical Engineering & Technology* 35, no. 7 Special Issue: SI (July 2012): 1281–1290, DOI: 10.1002/ceat.201100649.

Biedrzycki, Stephen; Buric, Michael P.; Falk, Joel; Woodruff, Steven D. "Angular output of hollow, metal-lined, waveguide Raman sensors." *Applied Optics* 51, no. 12 (April 2012): 2023–2025.

Boswell, Ray; Collett, Timothy S.; Frye, Matthew; Shedd, William; McConnell, Daniel R.; Shelander, Dianna. "Subsurface gas hydrates in the northern Gulf of Mexico." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 4–30, DOI: 10.1016/j.marpetgeo.2011.10.003.

Boswell, Ray; Frye, Matthew; Shelander, Dianna; Shedd, William; McConnelle, Daniel R.; Cook, Ann. "Architecture of gas-hydrate-bearing sands from Walker Ridge 313, Green Canyon 955, and Alaminos Canyon 21: Northern deepwater Gulf of Mexico." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 134–149, DOI: 10.1016/j.marpetgeo.2011.08.010.

Breault, Ronald W. "SELECTED PAPERS FROM THE 2010 NETL MULTIPHASE FLOW WORKSHOP Preface." *Powder Technology* 220, Special Issue SI, (April 2012): 1–1, DOI: 10.1016/j.powtec.2011.10.035.

Breault, Ronald W.; Casleton, Emily M.; Guenther, Christopher P. "Chaotic and statistical tests on fiber optic dynamic data taken from the riser section of a circulating fluidized bed." *Powder Technology* 220, Special Issue: SI (April 2012): 151–163, DOI: 10.1016/j.powtec.2011.09.002.

Brenner, Thomas A.; Fontenot, Raymond L.; Cizmas, Paul G. A.; O'Brien, Thomas J.; Breault, Ronald W. "A reduced-order model for heat transfer in multiphase flow and practical aspects of the proper orthogonal decomposition." *Computers & Chemical Engineering* 43 (August 2012): 68–80, DOI: 10.1016/j.compchemeng.2012.04.003.

Burgess, Ward A.; Tapriyal, Deepak; Morreale, Bryan D.; Wu, Yue; McHugh, Mark A.; Baled, Hseen; Enick, Robert M. "Prediction of fluid density at extreme conditions using the perturbed-chain SAFT equation correlated to high temperature, high pressure density data." *Fluid Phase Equilibria* 319 (April 2012): 55–56, DOI: 10.1016/j.fluid.2012.01.032.

Buric, Michael P.; Chorpening, Benjamin T.; Mullen, Jessica C.; Ranalli, Joseph A.; Woodruff, Steven D. "Field testing the Raman gas composition sensor for gas turbine operation." *Fiber Optic Sensors and Applications IX*, Book Series: Proceedings of *SPIE* 8370, Article Number 837009 (2012) DOI: 10.1117/12.919666.

Chao, Robin; Munprom, Ratiporn; Petrova, Rumyana; Gerdes, Kirk; Kitchin, John R.; Salvador, Paul A. "Structure and Relative Thermal Stability of Mesoporous (La,Sr) MnO_3 Powders Prepared Using Evaporation-Induced Self-Assembly Methods." *Journal of the American Ceramic Society* 95, no. 7 (July 2012): 2339–2346, DOI: 10.1111/j.1551-2916.2012.05236.x.

Chapman, Elizabeth C.;Capo, Rosemary C.;Stewart, Brian W.; Kirby, Carl S.; Hammack, Richard W.; Schroeder, Karl T.; Edenborn, Harry M. "Geochemical and Strontium Isotope Characterization of Produced Waters from Marcellus Shale Natural Gas Extraction." *Environmental Science & Technology* 46, no. 6 (March 2012): 3545–3553, DOI: 10.1021/es204005g.

Chen, De-Li; Al-Saidi, W. A.; Johnson, J. Karl. "Noble gases on metal surfaces: Insights on adsorption site preference." *Physical Review B* 84, no. 24, Article Number: 241405, (December 2011): DOI: 10.1103/PhysRevB.84.241405.

Chen, Ruey-Hung; Li, Zhiliang; Phuoc, Tran X."Propagation and stability characteristics of laminar lifted diffusion flame base." *Combustion and Flame* 159, no. 5 (May 2012): 1821–1831, DOI: 10.1016/j.combustflame.2012.01.016.

Chen, Song; Chen, Yun; Finklea, Harry; Song, Xueyan; Hackett, Gregory; Gerdes, Kirk. "Crystal defects of yttria stabilized zirconia in Solid Oxide Fuel Cells and their evolution upon cell operation." *Solid State Ionics* 206 (January 2012): 104–111, DOI: 10.1016/j.ssi.2011.11.008.

Chen, Yun; Chen, Song; Hackett, Gregory; Harry; Song, Xueyan; Gerdes, Kirk. "Microstructural and chemical evolution near anode triple phase boundary in Ni/YSZ solid oxide fuel cells." *Solid State Ionics* 204 (December 2011): 87–90, DOI: 10.1016/j.ssi.2011.10.005.

Collett, T. S.; Boswell, R.; Lee, M. W.; Anderson, B. J.; Rose, K.; Lewis, K. A. "Evaluation of Long-Term Gas-Hydrate-Production Testing Locations on the Alaska North Slope." *SPE Reservoir Evaluation & Engineering* 15, no. 2 (April 2012): 243–264.

Collett, Timothy S.; Boswell, Ray. "Resource and hazard implications of gas hydrates in the Northern Gulf of Mexico: Results of the 2009 Joint Industry Project Leg II Drilling Expedition Preface." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 1–3, DOI: 10.1016/j.marpetgeo.2012.01.002.

Cummings, Stephen; Xing, Dazun; Enick, Robert; Rogers, Sarah; Heenan, Richard; Grillo, Isabelle; Eastoe, Julian. "Design principles for supercritical CO_2 viscosifiers." *Soft Matter* 8, no. 26 (2012): 7044–7055, DOI: 10.1039/c2sm25735a.

Cygan, Randall T.; Romanov, Vyacheslav N.; Myshakin, Evgeniy M. "Molecular Simulation of Carbon Dioxide Capture by Montmorillonite Using an Accurate and Flexible Force Field." *Journal of Physical Chemistry C* 116, no. 24 (June 2012): 13079–13091, DOI: 10.1021/jp3007574.

Dikshit, Vivek; Yueh, Fang-Yu; Singh, Jagdish P.; McIntyre, Dustin L.; Jain, Jinesh C.; Melikechi, Nouredine. "Laser induced breakdown spectroscopy: A potential tool for atmospheric carbon dioxide measurement." *Spectrochimica Acta* Part B-Atomic Spectroscopy 68, no. 65–70 (February 2012): DOI: 10.1016 /j.sab.2012.01.009.

Dillon, Shen J.; Helmick, Lam; Miller, Herbert M.; Wilson, Lane; Gemman, Randall; Petrova, Rumyana V.; Barmak, Katayun; Rohrer, Gregory S.; Salvador, Paul A."The Orientation Distributions of Lines, Surfaces, and Interfaces around Three-Phase Boundaries in Solid Oxide Fuel Cell Cathodes." *Journal of the American Ceramic Society* 94, no. 11 (November 2011): 4045–4051, DOI: 10.1111/j.1551-2916.2011.04673.x.

Ding, Mengning; Sorescu, Dan C.; Kotchey, Gregg P.; Star, Alexander. "Welding of Gold Nanoparticles on Graphitic Templates for Chemical Sensing." *Journal of the American Chemical Society* 134, no. 7 (February 2012): 3472–3479, DOI: 10.1021/ja210278u.

Ding, Mengning; Star, Alexander. "Selecting Fruits with Carbon Nanotube Sensors." *Angewandte Chemie-International Edition* 51, no. 31(2012): 7637–7638, DOI: 10.1002/anie.201203387.

Dogan, Oe. N.; Hu, R.; Song, X.; Chen, S.; Gao, M. C. "Ordered bcc phases in a Cu-Pd-Mg hydrogen separation membrane alloy." *Journal of Alloys and Compounds* 528 (July 2012): 10–15, DOI: 10.1016/j.jallcom.2012.02.120.

Drese, Jeffrey H.; Choi, Sunho; Didas, Stephanie A.; Bollini, Praveen; Gray, McMahan L.; Jones, Christopher W. "Effect of support structure on CO_2 adsorption properties of pore-expanded hyperbranched aminosilicas." *Microporous and Mesoporous Materials* 151 (March 2012): 231–240, DOI: 10.1016/j.micromeso.2011.10.031.

Duan, Yuhua. "A first-principles density functional theory study of the electronic structural and thermodynamic properties of M_2ZrO_3 and M_2CO_3 (M=Na, K) and their capabilities for CO_2 capture." *Journal of Renewable and Sustainable Energy* 4, no. 1, Article Number: 013109 (January 2012): DOI: DOI: 10.1063/1.3683519.

Duan, Yuhua; Luebke, David R.; Pennline, Henry W.; Li, Bingyun; Janik, Michael J.; Halley, J. Woods. "Ab Initio Thermodynamic Study of the CO_2 Capture Properties of Potassium Carbonate Sesquihydrate, K_2CO_3 center dot 1.5H(2)O." *Journal of Physical Chemistry C* 116, no. 27 (July 2012): 14461–14470, DOI: 10.1021/jp303844t.

Epur, R; Ramanathan, M; Beck, FR; Manivannan, A; Kumta, PN. "Electrodeposition of amorphous silicon anode for lithium ion batteries." *Materiels Science and Engineering B-Advanced Functional Solid-State Materials* 177, no. 14 (August 2012): 1151-1156, DOI: 10.1016/j.mseb.2012.04.027.

Espinal, Laura; Morreale, Bryan D. "Materials challenges in carbon-mitigation technologies." *MRS Bulletin* 37, no. 4 (April 2012): 431–438, DOI: 10.1557/mrs.2012.10.

Fang, H. Z.; Wang, W. Y.; Jablonski, Paul D.; Liu, Z. K. "Effects of reactive elements on the structure and diffusivity of liquid chromia: An ab initio molecular dynamics study." *Physical Review B* 85, no. 1, Article Number: 014207(January 2012): DOI: 10.1103/PhysRevB.85.014207.

Fang, H. Z.; Wang, Y.; Shang, S. L.; Jablonski, Paul D.; Liu, Z. K. "First-principles calculations of interfacial and segregation energies in alpha-Cr_2O_3." *Journal of Physics-Condensed Matter* 24, no. 22, Article Number: 225001 (June 2012): DOI: 10.1088/0953-8984/24/22/225001.

Fauth, D. J.; Gray, M. L.; Pennline, H. W.; Krutka, H. M.; Sjostrom, S.; Ault, A. M. "Investigation of Porous Silica Supported Mixed-Amine Sorbents for Post-Combustion CO_2 Capture." *Energy & Fuels* 26, no. 4 (April 2012): 2483–2496, DOI: 10.1021/ef201578a.

Ferer, M.; Smith, D. H. "Characterising the Correlations of Failure Events: A 2-D Block-and-Springs Model." *Strain* 47, Supplement: 2 (December 2011): 187–195, DOI: 10.1111/j.1475-1305.2010.00758.x.

Fisher, James C., II; Siriwardane, Ranjani V.; Stevens, Robert W., Jr. "Process for CO_2 Capture from High-Pressure and Moderate-Temperature Gas Streams." *Industrial & Engineering Chemistry Research* 51, no. 14 (April 2012): 5273–5281, DOI: 10.1021/ie2022465.

Fisher, James C., II; Siriwardane, Ranjani V.; Stevens, Robert W., Jr. "Zeolite-Based Process for CO_2 Capture from High-Pressure, Moderate-Temperature Gas Streams." *Industrial & Engineering Chemistry Research* 50, no. 24 (December 2011): 13962–13968, DOI: 10.1021/ie201666g.

Frye, Matthew; Shedd, William; Boswell, Ray. "Gas hydrate resource potential in the Terrebonne Basin, Northern Gulf of Mexico." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 150–168, DOI: 10.1016/j.marpetgeo.2011.08.001.

Gao, Michael C. "Computational Thermodynamic and Kinetic Modeling of High-Entropy Alloys and Amorphous Alloys." ***JOM*** 64, no. 7 (July 2012): 828–829, DOI: 10.1007/s11837-012-0363-8.

Garg, Rahul; Galvin, Janine; Li, Tingwen; Pannala, Sreekanth. "Open-source MFIX-DEM software for gas-solids flows: Part I-Verification studies." *Powder Technology* 220, Special Issue: SI, (April 2012): 122–137, DOI: 10.1016/j.powtec.2011.09.019.

Gaur, Sarthak; Pakhare, Devendra; Wu, Hongyi; Haynes, Daniel J.; Spivey, James J. "CO_2 Reforming of CH_4 over Ru-Substituted Pyrochlore Catalysts: Effects of Temperature and Reactant Feed Ratio." *Energy & Fuels* 26, no. 4 (April 2012): 1989–1998, DOI: 10.1021/ef300158y.

Gong, Mingyang; Gemmen, Randall S.; Liu, Xingbo. "Modeling of oxygen reduction mechanism for 3PB and 2PB pathways at solid oxide fuel cell cathode from multi-step charge transfer." *Journal of Power Sources* 201(March 2012): 204–218, DOI: 10.1016/j.jpowsour.2011.11.002.

Gopalan, Balaji; Shaffer, Franklin. "A new method for decomposition of high speed particle image velocimetry data." *Powder Technology* 220, Special Issue: SI (April 2012): 164–171, DOI: 10.1016/j.powtec.2011.09.001.

Hackett, Gregory A.; Gerdes, Kirk; Song, Xueyan; Chen, Yun; Shuthanandan, Vaithiyalingam; Engelhard, Mark; Zhu, Zihua; Thevuthasan, Suntharampillai. "Performance of solid oxide fuel cells operated with coal syngas provided directly from a gasification process." *Journal of Power Sources* 214 (September 2012): 142–152 DOI: 10.1016/j.jpowsour.2012.04.050.

Helminiak, M. A.; Yanar, N. M.; Pettit, F. S.; Taylor, T. A.; Meier, G. H. "The effect of superalloy substrate on the behaviour of high-purity low-density air plasma sprayed thermal barrier coatings." *Materials at High Temperatures* 29, no. 3 (August 2012): 264–271, DOI: 10.3184/096034012X13335310236212.

Holloway, William; Benyahia, Sofiane; Hrenya, Christine M.; Sundaresan, Sankaran. "Meso-scale structures of bidisperse mixtures of particles fluidized by a gas." *Chemical Engineering Science* 66, no. 19, Special Issue: SI (October 2011): 4403–4420, DOI: DOI: 10.1016/j.ces.2011.05.037.

Huang, Rui; Patwardhan, Sachin C.; Biegler, Lorenz T. "Robust stability of nonlinear model predictive control based on extended Kalman filter." *Journal of Process Control* 22, no. 1 (January 2012): 82–89, DOI: 10.1016/j.jprocont.2011.10.006.

Huang, Ye; Gellman, Andrew J."Enantiospecific Adsorption of (R)-3-Methylcyclohexanone on Naturally Chiral Surfaces Vicinal to Cu(110)." *Topics in Catalysis* 54, no. 19-20, (December 2011): 1403–1413, DOI: 10.1007/s11244-011-9756-0.

Ipus, J. J.; Herre, P.; Ohodnicki, P.; McHenry, M. E. "High temperature x-ray diffraction determination of the body-centered-cubic-face-centered-cubic transformation temperature in $(Fe_70Ni_30)(88)Zr_7B_4Cu_1$ nanocomposites." *Journal of Applied Physics* 111, no. 7, Article Number: 07A323 (April 2012): DOI: 10.1063/1.3675990.

Jablonski, Paul D.; Hawk, Jeffery A.; Cowen, Christopher J.; Maziasz, Philip J. "Processing of Advanced Cast Alloys for A-USC Steam Turbine Applications." *JOM* 64, no. 2 (February 2012): 271–279, DOI: 10.1007/s11837-012-0241-4.

Jones, Dustin; Bhattacharyya, Debangsu; Turton, Richard; Zitney, Stephen E. "Rigorous Kinetic Modeling and Optimization Study of a Modified Claus Unit for an Integrated Gasification Combined Cycle (IGCC) Power Plant with CO_2 Capture." *Industrial & Engineering Chemistry Research* 51, no. 5 (February 2012): 2362–2375, DOI: 10.1021/ie201713n.

Kadakia, Karan; Datta, Moni Kanchan; Velikokhatnyi, Oleg I.; Jampani, Prashanth; Park, Sung Kyoo; Saha, Partha; Poston, James A.; Manivannan, Ayyakkannu; Kumta, Prashant N. "Novel (Ir,Sn,Nb)O-2 anode electrocatalysts with reduced noble metal content for PEM based water electrolysis." *International Journal of Hydrogen Energy* 37, no. 4 (February 2012): 3001–3013, DOI: 10.1016/j.ijhydene.2011.11.055.

Kaneko, Tetsuya K.; Zhu, Jingxi; Thomas, Hugh; Bennett, James P.; Sridhar, Seetharaman. "Influence of Oxygen Partial Pressure on Synthetic Coal Slag Infiltration into Porous Al_2O_3 Refractory." *Journal of the American Ceramic Society* 95, no. 5 (May 2012): 1764–1773, DOI: 10.1111/j.1551-2916.2012.05175.x.

Kaneko, Tetsuya Kenneth; Bennett, James P.; Sridhar, Seetharaman. "Effect of Temperature Gradient on Industrial Gasifier Coal Slag Infiltration into Alumina Refractory." *Journal of the American Ceramic Society* 94, no. 12 (December 2011): 4507–4515, DOI: 10.1111/j.1551-2916.2011.04782.x.

Kasule, Job S.; Turton, Richard; Bhattacharyya, Debangsu; Zitney, Stephen E. "Mathematical Modeling of a Single-Stage, Downward-Firing, Entrained-Flow Gasifier." *Industrial & Engineering Chemistry Research* 51, no. 18 (May 2012): 6429–6440, DOI: 10.1021/ie202121h.

Kauffman, Douglas R; Alfonso, Dominic; Matranga, Christopher; Qian, Huifeng; Jin, Rongchao. "Experimental and Computational Investigation of Au-25 Clusters and CO_2: A Unique Interaction and Enhanced Electrocatalytic Activity." *Journal of the American Chemical Society* 134, no. 24 (June 2012): 10237–10243, DOI: 10.1021/ja303259q.

Kernion, Samuel J.; Ohodnicki, Paul R.; McHenry, Michael E. "In-situ investigation of phase formation in nanocrystalline $(Co_{97.5}Fe_{2.5})(89)Zr_7B_4$ alloy by high temperature x-ray diffraction." *Journal of Applied Physics* 111, no. 7, Article Number: 07A316 (April 2012): DOI: 10.1063/1.3673433.

Kim, Jeongho; Massoudi, Mehrdad; Antaki, James F.; Gandini, Alberto. "Removal of malaria-infected red blood cells using magnetic cell separators: A computational study." *Applied Mathematics and Computation* 218, no. 12 (February 2012): 6841–6850, DOI: 10.1016/j.amc.2011.12.057.

Konda, N. V. S. N. Murthy; Shah, Nilay; Brandon, Nigel P. "Dutch hydrogen economy: evolution of optimal supply infrastructure and evaluation of key influencing elements." *Asia-Pacific Journal of Chemical Engineering* 7, no. 4 (July-August 2012):: 534–546, DOI: 10.1002/apj.604.

Ksepko, Ewelina; Siriwardane, Ranjani V.; Tian, Hanjing; Simonyi, Thomas; Sciazko, Marek. "Effect of H_2S on Chemical Looping Combustion of Coal-Derived Synthesis Gas over Fe-Mn Oxides Supported on Sepiolite, ZrO_2, and Al_2O_3." *Energy & Fuels* 25, no. 4 (April 2012): 2461–2472, DOI: 10.1021/ef201441k.

Lamont, Justin A.; Ekkad, Srinath V.; Alvin, Mary Anne. "Effects of Rotation on Heat Transfer for a Single Row Jet Impingement Array with Crossflow." *Journal of Heat Transfer-Transactions of ASME* 134, no. 8, Article Number: 082202 (August 2012): DOI: 10.1115/1.4006167.

Lawton, T. J.; Pushkarev, V.; Broitman, E.; Reinicker, A; Sykes, E. C. H.; Gellman, A. J. "Initial Oxidation of Cu(hkl) Surfaces Vicinal to Cu(111): A High-Throughput Study of Structure Sensitivity." *Journal of Physical Chemistry C* 116, no. 30 (August 2012): 16054–16062, DOI: 10.1021/jp303488t.

Leary, Alex M.; Ohodnicki, Paul R.; McHenry, Michael E. "Soft Magnetic Materials in High-Frequency, High-Power Conversion Applications." *JOM* 64, no. 7 (July 2012): 772–281, DOI: 10.1007/s11837-012-0350-0.

Lee, Junseok; Sorescu, Dan C.; Deng, Xingyi; Jordan, Kenneth D. "Diffusion of CO_2 on the Rutile TiO_2(110) Surface." *Journal of Physical Chemistry Letters* 2, no. 24 (December 2011): 3114–3117, DOI: 10.1021/jz201339n.

Lee, Shiwoo; Miller, Nicholas; Gerdes, Kirk. "Long-Term Stability of SOFC Composite Cathode Activated by Electrocatalyst Infiltration." *Journal of the Electrochemical Society* 159, no. 7 (2012): F301–F308, DOI: 10.1149/2.067207jes.

Lee, Shiwoo; Miller, Nicholas; Staruch, Margo; Gerdes, Kirk; Jain, Menka; Manivannan, Ayyakkannu. "$Pr_{0.6}Sr_{0.4}CoO_3$-delta electrocatalyst for solid oxide fuel cell cathode introduced via infiltration." *Electrochimica Acta* 56, no. 27 (November 2011): 9904–9909, DOI: 10.1016/j.electacta.2011.08.060.

Lekse, Jonathan W.; Underwood, M. Kylee; Lewis, James P.; Matranga, Christopher. "Synthesis, Characterization, Electronic Structure, and Photocatalytic Behavior of $CuGaO_2$ and $CuGa_{1-x}Fe_xO_2$ (x=0.05, 0.10, 0.15, 0.20) Delafossites." *Journal of Physical Chemistry C* 116, no. 2 (January 2012): 1865–1872, DOI: 10.1021/jp2081225.

Li, Dan; Han, Ju-Guang; Chen, Hang; Li, Liang; Zhao, Run-Ning; Liu, Guang; Duan, Yuhua. "Insights into the structural function of the complex of HIV-1 protease with TMC-126: molecular dynamics simulations and free-energy calculations." *Journal of Molecular Modeling* 18, no. 5 (May 2012): 1841–1854, DOI: 10.1007/s00894-011-1205-2.

Li, Qun; Liang, Linyun; Gerdes, Kirk; Chen, Long-Qing. "Phase-field modeling of three-phase electrode microstructures in solid oxide fuel cells." *Applied Physics Letters* 101, no. 3, Article Number 033909 (July 2012): DOI: 10.1063/1.4738230.

Li, Tingwen; Benyahia, Sofiane. "Revisiting Johnson and Jackson boundary conditions for granular flows." *AIChE Journal* 58, no. 7 (July 2012): 2058–2068, DOI: 10.1002/aic.12728.

Li, Tingwen; Dietiker, Jean-Francois; Zhang, Yongmin; Shahnam, Mehrdad. "Cartesian grid simulations of bubbling fluidized beds with a horizontal tube bundle." *Chemical Engineering Science* 66, no. 23 (December 2011): 6220–6231, DOI: 10.1016/j.ces.2011.08.056.

Li, Tingwen; Garg, Rahul; Galvin, Janine; Pannala, Sreekanth. "Open-source MFIX-DEM software for gas-solids flows: Part II - Validation studies." *Powder Technology* 220, Special Issue: SI (April 2012): 138–150, DOI: 10.1016/j.powtec.2011.09.020.

Li, Tingwen; Grace, John; Shadle, Lawrence; Guenther, Chris. "On the superficial gas velocity in deep gas-solids fluidized beds." *Chemical Engineering Science* 66, no. 22 (November 2011): 5735-5738, DOI: 10.1016/j.ces.2011.08.002.

Li, Tingwen; Guenther, Chris. "A CFD study of gas-solid jet in a CFB riser flow." *AIChE Journal* 58, no. 3 (March 2012): 756–769, DOI: 10.1002/aic.12619.

Li, Tingwen; Guenther, Chris. "MFIX-DEM simulations of change of volumetric flow in fluidized beds due to chemical reactions." *Powder Technology* 220, Special Issue: SI (April 2012): 70–78, DOI: 10.1016/j.powtec.2011.09.025.

Li, Yihong; Gerdes, Kirk; Diamond, Harvey; Liu, Xingbo. "An improved method to increase the predictive accuracy of the ECR technique." *Solid State Ionics* 204 (December 2012): 104–110, DOI: 10.1016/j.ssi.2011.09.017.

Liu, Faye; Lu, Peng; Griffith, Craig; Hedges, Sheila W.; Soong, Yee; Hellevang, Helge; Zhu, Chen. "CO_2-brine-caprock interaction: Reactivity experiments on Eau Claire shale and a review of relevant literature." *International Journal of Greenhouse Gas Control* 7 (March 2012): 153– 167, DOI: 10.1016/j.ijggc.2012.01.012.

Liu, Yong; Gamwo, Isaac K. "Comparison between equilibrium and kinetic models for methane hydrate dissociation." *Chemical Engineering Science* 69, no. 1 (February 2012): 193–200, DOI: 10.1016/j.ces.2011.10.020.

Lu, Jiemin; Kharaka, Yousif K.; Thordsen, James J.; Horita, Juske; Karamalidis, Athanasios; Griffith, Craig; Hakala, J. Alexandra; Ambats, Gil; Cole, David R.; Phelps, Tommy J.; Manning, Michael A.; Cook, Paul J.; Hovorka, Susan D. "CO_2-rock-brine interactions in Lower Tuscaloosa Formation at Cranfield CO_2 sequestration site, Mississippi, USA." *Chemical Geology* 291 (January 2012): 269–277, DOI: 10.1016/j.chemgeo.2011.10.020.

Malkhandi, S.; Yang, B.; Manohar, A. K.; Manivannan, A.; Prakash, G. K. Surya; Narayanan, S. R. "Electrocatalytic Properties of Nanocrystalline Calcium-Doped Lanthanum Cobalt Oxide for Bifunctional Oxygen Electrodes." *Journal of Physical Chemistry Letters* 3, no. 8 (April 2012): 967–972, DOI: 10.1021/jz300181a.

Mandeltort, Lynn; Choudhury, Pabitra; Johnson, J. Karl; Yates, John T., Jr. "Methyl Radical Reactivity on the Basal Plane of Graphite." *Journal of Physical Chemistry C* 116, no. 34 (August 2012): 18347–18357, DOI: 10.1021/jp3063367.

Mandeltort, Lynn; Choudhury, Pabitra; Johnson, J. Karl; Yates, John T., Jr. "Reaction of the Basal Plane of Graphite with the Methyl Radical." *Journal of Physical Chemistry Letters* 3, no. 12 (June 2012): 1680-1683, DOI: 10.1021/jz300578x.

Massoudi, Mehrdad; Kim, Jeongho; Antaki, James F. "Modeling and numerical simulation of blood flow using the theory of interacting continua." *International Journal of Non-linear Mechanics* 47, no. 5 (June 2012): 506–520, DOI: 10.1016/j.ijnonlinmec.2011.09.025.

Massoudi, Mehrdad; Phuoc, Tran X. "Remarks on Constitutive Modeling of Nanofluids." *Advances in Mechanical Engineering*. Article Number: 927580 (2012): DOI: 10.1155/2012/927580.

Massoudi, Mehrdad; Vaidya, Ashwin. "Analytical solutions to Stokes-type flows of inhomogeneous fluids." *Applied Mathematics and Computation* 218, no. 11 (February 2012): 6314–6329, DOI: 10.1016/j.amc.2011.11.110.

Mastalerz, Maria; Goodman, Angela; Chirdon, Danielle. "Coal Lithotypes before, during, and after Exposure to CO_2: Insights from Direct Fourier Transform Infrared Investigation." *Energy & Fuels* 26, no. (June 2012): 3586–3591, DOI: 10.1021/ef3003813.

McConnell, Daniel R.; Zhang, Zijian; Boswell, Ray. "Review of progress in evaluating gas hydrate drilling hazards." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 209–223, DOI: 10.1016/j.marpetgeo.2012.02.010.

McGann, John P.; Zhong, Mingjiang; Kim, Eun Kyung; Natesakhawat, Sittichai; Jaroniec, Mietek; Whitacre, Jay F.; Matyjaszewski, Krzysztof; Kowalewski, Tomasz. "Block Copolymer Templating as a Path to Porous Nanostructured Carbons with Highly Accessible Nitrogens for Enhanced (Electro) chemical Performance." *Macromolecular Chemistry and Physics* 213, no. 10-11, Special Issue: SI (June 2012): 1078–1090, DOI: 10.1002/macp.201100691.

Michalak, W. D.; Miller, J. B.; Alfonso, D. R.; Gellman, A. J. "Uptake, transport, and release of hydrogen from Pd(100)." *Surface Science* 606, no. 304 (February 2012): 146–155, DOI: 10.1016/j.susc.2011.08.022.

Miller, Duane D.; Siriwardane, Ranjani; Simonyi, Thomas. "Theoretical and Experimental Analysis of Oxygen Separation from Air over Ni-Transition Metal Complexes." *Energy & Fuels* 25, no. 10 (October 2011): 4261–4270, DOI: 10.1021/ef200779m.

Miller, Matthew B.; Bing, Wei; Luebke, David R.; Enick, Robert M. "Solid CO_2-philes as potential phase-change physical solvents for CO_2." *Journal of Supercritical Fluids* 61 (January 2012): 212–220, DOI: 10.1016/j.supflu.2011.09.003.

Minsley, Burke J.; Smith, Bruce D.; Hammack, Richard; Sams, James I.; Veloski, Garret. "Calibration and filtering strategies for frequency domain electromagnetic data." *Journal of Applied Geophysics* 80 (May 2012): 55–56, DOI: 10.1016/j.jappgeo.2012.01.008.

Mohaghegh, Shahab D.; Gruic, Ognjen; Zargari, Saeed; Kalantari-Dahaghi, Amirmasoud; Bromhal, Grant S. "Top-down, intelligent reservoir modelling of oil and gas producing shale reservoirs: case studies." *International Journal of Oil Gas and Coal Technology* 5, no. 1 (2012): 3–28.

Monazam, Esmail R.; Shadle, Lawrence J.; Siriwardane, Ranjani. "Equilibrium and Absorption Kinetics of Carbon Dioxide by Solid Supported Amine Sorbent." *AIChE Journal* 51, no. 11 (November 2011): 3153–3159, DOI: 10.1002/aic.12516.

Monazam, Esmail R.; Shadle, Lawrence J.; Siriwardane, Ranjani. "Performance and Kinetics of a Solid Amine Sorbent for Carbon Dioxide Removal." *Industrial & Engineering Chemistry Research* 50, no. 19 (October 2011): 10989–10995, DOI: 10.1021/le201214q.

Monazam, Esmail R.; Siriwardane, Ranjani; Breault, Ronald W.; Tian, Hanjing; Shadle, Lawrence J.; Richards, George; Carpenter, Stephen. "Kinetics of the Reduction of CuO/Bentonite by Methane (CH_4) during Chemical Looping Combustion." *Energy & Fuels* 26, no. 5 (May 2012): 2779–2785, DOI: 10.1021/ef300072d.

Myshakin, Evgeniy M.; Gaddipati, Manohar; Rose, Kelly; Anderson, Brian J. "Numerical simulations of depressurization-induced gas production from gas hydrate reservoirs at the Walker Ridge 313 site, northern Gulf of Mexico." *Marine and Petroleum Geology* 34, no. 1, (June 2012): 169–185, DOI: 10.1016/j.marpetgeo.2011.09.001.

Nielsen, Benjamin C.; Gerdes, Kirk; O'Connor, William; Song, Xueyan; Abernathy, Harry. "Partitioning of coal contaminants in the components of liquid tin anode solid oxide fuel cells." *Journal of Power Sources* 211 (August 2012): 192–201, DOI: 10.1016/j.jpowsour.2012.03.057.

O'Brien, Casey P.; Miller, James B.; Morreale, Bryan D.; Gellman, Andrew J. "The Kinetics of H_2-D_2 Exchange over Pd, Cu, and PdCu Surfaces." *Journal of Physical Chemistry C* 115, no. 49 (December 2011): 24221–24230, DOI: 10.1021/jp2076885.

Ogretim, Egemen; Mulkeen, Everett; Gray, Donald D., Bromhal, Grant S. "A parametric study of the transport of CO_2 in the near-surface." *International Journal of Greenhouse Gas Control* 9 (July 2012): 294–302, DOI: 10.1016/j.ijggc.2012.04.007.

Ohodnicki, Paul R., Jr.; Natesakhawat, Sittichai; Baltrus, John P.; Howard, Bret; Brown, Thomas D. "Characterization of optical, chemical, and structural changes upon reduction of sol-gel deposited SnO_2 thin films for optical gas sensing at high temperatures." *Thin Solid Films* 520, no. 19 (July 2012): 6243–6249, DOI: 10.1016/j.tsf.2012.05.023.

Ohodnicki, Paul R., Jr.; Wang, Congjun; Natesakhawat, Sittichai; Baltrus, John P.; Brown, Thomas D. "In-situ and ex-situ characterization of TiO_2 and Au nanoparticle incorporated TiO_2 thin films for optical gas sensing at extreme temperatures." *Journal of Applied Physics* 111, no. 6, Article Number 064320 (March 2012): DOI: 10.1063/1.3695380.

Pekney, Natalie; Wells, Arthur; Diehl, J. Rodney; McNeil, Matthew; Lesko, Natalie; Armstrong, James; Ference, Robert. "Atmospheric monitoring of a perfluorocarbon tracer at the 2009 ZERT Center experiment." *Atmospheric Environment* 47 (February 2012): 124–132, DOI: 10.1016/j.atmosenv.2011.11.024.

Perry, Robert J.; Wood, Benjamin R.; Genovese, Sarah; O'Brien, Michael J.; Westendorf, Tiffany; Meketa, Matthew L.; Farnum, Rachel; McDermott, John; Sultanova, Irina; Perry, Thomas M.; Vipperla, Ravi-Kumar; Wichmann, Lisa A.; Enick, Robert M.; Hong, Lei; Tapriyal, Deepak. "CO_2 Capture Using Phase-Changing Sorbents." *Energy & Fuels* 26, no. 4 (April 2012): 2528–2538, DOI: 10.1021/ef300079w.

Phuoc, Tran X.; Chen, Ruey-Hung. "Modeling the effect of particle size on the activation energy and ignition temperature of metallic nanoparticles." *Combustion and Flame* 159, no. 1 (January 2012): 416–419, DOI: 10.1016/j.combustflame.2011.07.003.

Poulston, Stephen; Granite, Evan J.; Pennline, Henry W.; Hamilton, Hugh; Smith, Andrew W. J. "Palladium based sorbents for high temperature arsine removal from fuel gas." *Fuel* 90, no. 10 (October 2011): 3118–3121, DOI: 10.1016/j.fuel.2011.05.012.

Priyadarshini, Deepika; Kondratyuk, Petro; Miller, James B.; Gellman, Andrew J. "Compact tool for deposition of composition spread alloy films." *Journal of Vacuum Science & Technology A* 30, no. 1, Article Number: 011503 (January 2012): DOI: 10.1116/1.3664078.

Ranalli, Joseph; Ferguson, Don. "Measurement of Flame Frequency Response Functions Under Exhaust Gas Recirculation Conditions." *Journal of Engineering for Gas Turbines and Power-Transactions of the ASME* 134, no. 9, Article Number: 091502 (September 2012): DOI: 10.1115/1.4006877.

Rhodes, William D.; Kovalchuk, Vladimir I.; McDonald, Mark A. "Reaction pathways of halocarbon catalytic oligomerization." *Catalysis Communications* 18, no. 98–101 (February 2012): DOI: 10.1016/j.catcom.2011.11.019.

Rupp, Erik C.; Granite, Evan J.; Stanko, Dennis C. "Catalytic formation of carbonyl sulfide during warm gas clean-up of simulated coal-derived fuel gas with Pd/gamma-Al_2O_3 sorbents." *Fuel* 92, no. 1 (February 2012): 211–215, DOI: 10.1016/j.fuel.2011.06.055.

Salazar-Villalpando, Maria D. "Syn-gas generation in the absence of oxygen and isotopic exchange reactions over Rh & Pt/doped-ceria catalysts." *International Journal of Hydrogen Energy* 37, no. 3 (February 2012): 2121–2128, DOI: 10.1016/j.ijhydene. 2011.10.103.

Seehra, M. S.; Akkineni, L. P.; Yalamanchi, M.; Singh, V.; Poston, J. "Structural characteristics of nanoparticles produced by hydrothermal pretreatment of cellulose and their applications for electrochemical hydrogen generation." *International Journal of Hydrogen Energy* 37, no. 12 (June 2012): 9514–9523, DOI: 10.1016/j.ijhydene.2012.03.083.

Shedd, William; Boswell, Ray; Frye, Matthew; Godfriaux, Paul; Kramer, Kody. "Occurrence and nature of 'bottom simulating reflectors' in the northern Gulf of Mexico." *Marine and Petroleum Geology* 34, no. 1 (June 2012): 31–40, DOI: 10.1016/j.marpetgeo.2011.08.005.

Shi, Wei; Myers, Christina; Luebke, David R.; Steckel, Janice A.; Sorescu, Dan C. "Theoretical and Experimental Studies of CO_2 and H_2 Separation Using the 1-Ethyl-3-methylimidazolium Acetate ([emim][CH_3COO]) Ionic Liquid." *Journal of Physical Chemistry B* 116, no. 1 (January 2012): 283–295, DOI: 10.1021/jp205830d.

Shukla, Nisha; Ondeck, Abigail; Lee, Johanna C.; Miller, James B. "$NiFe_2O_4$@SiO_2 Nanoparticles Stabilized by Porous Silica Shells." *Catalysis Letters* 142, no. 5 (May 2012): 582–587; DOI: 10.1007/s10562-012-0795-3.

Siefert, Nicholas; Shekhawat, Dushyant; Litster, Shawn; Berry, David. "Molten catalytic coal gasification with in situ carbon and sulphur capture." *Energy & Environmental Science* 5, no. 9 (September 2012): 8660–8672 DOI: 10.1039/c2ee21989a.

Singh, Gurpreet; Thomas, R; Kumar, Arun; Katiyar, R. S.; Manivannan, A. "Electrochemical and Structural Investigations on ZnO Treated 0.5 Li_2MnO_3-0.5LiMn(0.5)Ni(0.5)O(2) Layered Composite Cathode Material for Lithium Ion Battery." *Journal of the Electrochemical Society* 159, no. 4 (2012): A470–A478, DOI: 10.1149/2.100204jes.

Singh, V.; Seehra, M. S.; Manivannan, A.; Kumta, P. N. "Magnetic characteristics of a new cubic defect spinel $Li_{0.5}Mg_{0.5}MnO_3$." *Journal of Applied Physics* 111, no. 7, Article Number 07E302 (April 2012): DOI: 10.1063/1.3670504.

Siriwardane, Hema J.; Bowes, Benjamin D.; Bromhal, Grant S.; Gondle, Raj K.; Wells, Arthur W.; Strazisar, Brian R. "Modeling of CBM production, CO_2 injection, and tracer movement at a field CO_2 sequestration site." *International Journal of Coal Geology* 96-97, no. 120–136 (July 2012): DOI: 10.1016/j.coal.2012.02.009.

Siw, Sin Chien; Chyu, Minking K.; Shih, Tom I-P.; Alvin, Mary Anne. "Effects of Pin Detached Space on Heat Transfer and Pin-Fin Arrays." *Journal of Heat Transfer-Transaction of the ASME* 134, no. 8, Article Number: 081902 (August 2012): DOI: 10.1115/1.4006166.

Son, You-Hwan; Lee, Jung-Kun; Soong, Yee; Martello, Donald; Chyu, Minking K. "Heterostructured zero valent iron-montmorillonite nanohybrid and their catalytic efficacy." *Applied Clay Science* 62-63, no. 21–26 (July 2012): DOI: .1016/j.clay.2012.04.003.

Soong, Yee; Dilmore, Robert M.; Hedges, Sheila W.; Howard, Bret H.; Romanov, Vyacheslav. "Utilization of Multiple Waste Streams for Acid Gas Sequestration and Multi-Pollutant Control." *Chemical Engineering & Technology* 35, no. 3, Special Issue: SI (March 2012): 473–481, DOI: 10.1002/ceat.201100341.

Sorescu, Dan C.; Lee, Junseok; Al-Saidi, Wissam A.; Jordan, Kenneth D. "Coadsorption properties of CO_2 and H_2O on TiO_2 rutile (110): A dispersion-corrected DFT study." *Journal of Chemical Physics* 137, no. 7, Article Number: 074704 (August 2012): DOI: 10.1063/1.

Spivak-Birndorf, Lev J.; Stewart, Brian W.; Capo, Rosemary C.; Chapman, Elizabeth C.; Schroeder, Karl T.; Brubaker, Tonya M. "Strontium Isotope Study of Coal Utilization By-Products Interacting with Environmental Waters." *Journal of Environmental Quality* 41, no. 1 (January 2012): 144–154, DOI: 10.2134/jeq2011.0222.

Subramanyan, Karthik; Diwekar, Urmila; Zitney, Stephen E. "Stochastic modeling and multi-objective optimization for the APECS system." *Computers & Chemical Engineering* 35, no. 12 (December 2011): 2667–2679, DOI: 10.1016/j.compchemeng.2011.02.003.

Syamlal, Madhava. "A hyperbolic model for fluid-solids two-phase flow." *Chemical Engineering Science* 66, no. 19, Special Issue: SI (October 2011): 4421-4425, DOI: 10.1016/j.ces.2011.02.051.

Thompson, Robert L.; Hedges, Sheila W. "Thermal stability study of the bridging CO_2 complex, [(Bu3P)-Bu-t-(mu-CO_2)-B(C6F5)(3)]." *Fuel* 95, no. 1 (May 2012): 655–658, DOI: 10.1016/j.fuel.2011.11.051.

Traverso, Alberto; Tucker, David; Haynes, Comas L. "Preliminary Experimental Results of Integrated Gasification Fuel Cell Operation Using Hardware Simulation." *Journal of Engineering for Gas Turbines and Power-Transactions of the ASME* 134, no. 7, Article Number: 071701 (July 2012): DOI: 10.1115/1.4005976.

Tsai, Alex; Tucker, David; Clippinger, David. "Simultaneous Turbine Speed Regulation and Fuel Cell Airflow Tracking of a SOFC/GT Hybrid Plant with the Use of Airflow Bypass Valves." *Journal of Fuel Cell Science and Technology* 8, no. 6, Article Number: 061018 (December 20110: DOI: 10.1115/1.4004643.

Tucker, David; VanOsdol, John; Liese, Eric; Lawson, Larry; Zitney, Stephen; Gemmen, Randall; Ford, J. Christopher; Haynes, Comas. "Evaluation of Methods for Thermal Management in a Coal-Based SOFC Turbine Hybrid Through Numerical Simulation." *Journal of Fuel Cell Science and Technology* 9, no. 4, Article Number 041004 (August 2012): DOI: 10.1115/1.4006044.

Vesper, Dorothy J.; Edenborn, Harry M. "Determination of free CO_2 in emergent groundwaters using a commercial beverage carbonation meter." *Journal of Hydrology* 438 (May 2012): 148–155, DOI: 10.1016/j.jhydrol.2012.03.015.

Wang, Yi; Fang, Huazhi; Zacherl, Chelsey L.; Mei, Zhigang; Shang, Shunli; Chen, Long-Qing'; Jablonski, Paul D.; Liu, Zi-Kui. "First-principles lattice dynamics, thermodynamics, and elasticity of Cr_2O_3." *Surface Science* 606, no. 17-18 (September 2012): 1422–1425, DOI: 10.1016/j.susc.2012.05.006.

Weiland, Nathan T.; Means, Nicholas C.; Morreale, Bryan D. "Product distributions from isothermal co-pyrolysis of coal and biomass." *Fuel* 94, no. 1 (April 2012): 563-570, DOI: 10.1016/j.fuel.2011.10.046.

Wen, You-Hai; Chen, Long-Qing; Hawk, Jeffrey A. "Phase-field modeling of corrosion kinetics under dual-oxidants." *Modeling and Simulation in Materials Science and Engineering* 20, no. 3, Article Number: 035013 (April 2012): DOI: 10.1088/0965-0393/20/3/035013.

Wilson, Thomas H.; Wells, Art; Peters; Dwight; Mioduchowski, Andrew; Martinez, Gabriela; Koperna, George; Akwari, Bill N.; Heath, Jason. "Fracture and 3-D seismic interpretations of the Fruitland Formation and cover strata: Implications for CO_2 retention and tracer movement, San Juan Basin Pilot test." *International Journal of Coal Geology* 99 (September 2012): 35–53, DOI: 10.1016/j.coal.2012.02.007.

Wu, Kaisheng; Dogan, Omer N.; Velikokhatnyi, Oleg I.; Kumta, Prashant N. "A CALPHAD study on the thermodynamic stability of calcium-, zinc-, and yttrium-doped magnesium in aqueous environments." *Materials Science and Engineering B-Advanced Functional Solid-State Materials* 176, no. 20, Special Issue: SI (December 2011): 1727–1732, DOI: 10.1016/j.mseb.2011.04.016.

Wu, Yue; Bamgbade, Babatunde; Liu, Kun; McHugh, Mark A.; Baled, Hseen; Enick, Robert M.; Burgess, Ward A.; Tapriyal, Deepak; Morreale, Bryan D. "Experimental measurements and equation of state modeling of liquid densities for long-chain n-alkanes at pressures to 265 MPa and temperatures to 523 K." *Fluid Phase Equilibria* 311 (December 2011): 17–24, DOI: 10.1016/j.fluid.2011.08.020.

Yang, Ya-Mei; Small, Mitchell J.; Junker, Brian; Bromhal, Grant S.; Strazisar, Brian; Wells, Arthur. "Bayesian hierarchical models for soil CO_2 flux and leak detection at geologic sequestration sites." *Environmental Earth Sciences* 64, no. 3, (October 2011): 787–798, DOI: 10.1007/s12665-011-0903-5.

Zhang, Bo; Duan, Yuhua; Johnson, Karl. "Density functional theory study of CO_2 capture with transition metal oxides and hydroxides." *Journal of Chemical Physics* 136, no. 6, Article Number: 064516 (February 2012): DOI: 10.1063/1.3684901.

Zhang, Bo; Sorescu, Dan C.; Johnson, J. Karl; Majzoub, Eric H.; Luebke, David R. "Density functional theory studies on the electronic, structural, phonon dynamical and thermo-stability properties of bicarbonates $MHCO_3$, M = Li, Na, K." *Journal of Physics-Condensed Matter* 24, no. 32, Article Number: 325501 (August 2012): DOI: 10.1088/0953-8984/24/32/325501.

Zhang, Guozhen; Al-Saidi, W. A.; Myshakin, Evgeniy M.; Jordan, Kenneth D. "Dispersion-Corrected Density Functional Theory and Classical Force Field Calculations of Water Loading on a Pyrophyllite(001) Surface." *Journal of Physical Chemistry C* 116, no. 32 (August 2012): 17134–17141, DOI: 10.1021/jp305801d.

Zhao, Xinyu; Haworth, D. C.; Huckaby, E. David. "Transported PDF Modeling of Nonpremixed Turbulent $CO/H_2/N_2$ Jet Flames." *Combustion Science and Technology* 184, no. 5 (2012): 676–693, DOI: 10.1080/00102202.2012.660223.

Zheng, Peng; Greve, David W.; Oppenheim, Irving J.; Chin, Tao-Lun; Malone, Vanessa. "Langasite Surface Acoustic Wave Sensors: Fabrication and Testing." *IEEE Transactions on Ultrasonics Ferroelectrics and Frequency Control* 59, no. 2 (February 2012): 295–303, DOI: 10.1109/TUFFC.2012.2190.

Zhi, Mingjia; Koneru, Anveeksh; Yang, Feng; Manivannan, Ayyakkannu; Li, Jing; Wu, Nianqiang. "Electrospun $La_{0.8}Sr_{0.2}MnO_3$ nanofibers for a high-temperature electrochemical carbon monoxide sensor." *Nanotechnology* 23, no. 30, Article Number: 305501 (August 2012): DOI: 10.1088/0957-4484/23/30/304=5501.

Zhi, Mingjia; Lee, Shiwoo; Miller, Nicholas; Menzler, Norbert H.; Wu, Nianqiang. "An intermediate-temperature solid oxide fuel cell with electrospun nanofiber cathode." *Energy & Environmental Science* 5, no. 5 (May 2012): 7066–7071, DOI: 10.1039/c2ee02619h.

Zhi, Mingjia; Manivannan, Ayyakkannu; Meng, Fanke; Wu, Nianqiang. "Highly conductive electrospun carbon nanofiber/MnO_2 coaxial nano-cables for high energy and power density supercapacitors." *Journal of Power Sources* 208, no. 345–353, DOI: 10.1016/j.jpowsour.2012.02.048.

Zhou, Zhong; Bhamare, Sagar; Ramakrishnan, Gokul; Mannava, Seetha R.; Langer, Kristina; Wen, Youhai; Qian, Dong; Vasudevan, Vijay K. "Thermal relaxation of residual stress in laser shock peened Ti-6Al-4V alloy." *Surface & Coatings Technology* 206, no. 22 (June 2012): 4619–4627, DOI: 10.1016/j.surfcoat.2012.05.022.

Zhu, Jingxi; Holcomb, Gordon R.; Jablonski, Paul D.; Wise, Adam; Li, Jia; Laughlin, David E.; Sridhar, Seetharaman. "Subsurface characterization of an oxidation-induced phase transformation and twinning in nickel-based superalloy exposed to oxy-combustion environments." *Materials Science and Engineering A-Structural-Materials Properties Microstructure and Processing* 550 (July 2012): 243–253, DOI: 10.1016/j.msea.2012.04.066.

Zhu, Jingxi; Kaneko, Tetsuya Kenneth; Mu, Haoyuan; Bennett, James P.; Sridhar, Seetharaman. "Effects of Measurement Materials and Oxygen Partial Pressure on the Viscosity of Synthetic Eastern and Western United States Coal Slags." *Energy & Fuels* 26, no. 7 (July 2012): 4465–4474, DOI: 10.1021/ef300632x.

Ziomek-Moroz, M. "Environmentally Assisted Cracking of Drill Pipes in Deep Drilling Oil and Natural Gas Wells." *Journal of Materials Engineering and Performance* 21, no. 6 (June 2012): 1061–1069, DOI: 10.1007/s11665-011-9956-6.

Ziomek-Moroz, M.; Jablonski, P. "Effects of Ceric Oxide Coatings on Materials Performance of 430 Steel in Coal Synthetic Gas." *Materials Performance* 50, no. 12 (December 2012): 40–44.

Zou, Chenyu; van Duin, Adri C. T.; Sorescu, Dan C. "Theoretical Investigation of Hydrogen Adsorption and Dissociation on Iron and Iron Carbide Surfaces Using the ReaxFF Reactive Force Field Method." *Topics in Catalysis* 55, no. 5-6 (June 2012): 391–401, DOI: 10.1007/s11244-012-9796-0.

NETL-RUA Contacts

Julianne Klara
NETL, NETL-RUA Manager
(412) 386-6089
Julianne.Klara@NETL.DOE.GOV

George Guthrie
NETL, Focus Area Lead
Geological & Environmental Systems
(412) 386-6571
George.Guthrie@NETL.DOE.GOV

Bryan Morreale
NETL, Acting Focus Area Lead
Materials Science & Engineering
(412) 386-5929
Bryan.Morreale@NETL.DOE.GOV

George Richards
NETL, Focus Area Lead
Energy System Dynamics
(304) 285-4458
George.Richards@NETL.DOE.GOV

Madhava Syamlal
NETL, Focus Area Lead
Computational and Basic Sciences
(304) 285-4685
Madhava.Syamlal@NETL.DOE.GOV

Richard A. Bajura
NETL-RUA Consortium Area Lead
West Virginia University
(304) 285-9999
Richard.Bajura@CONTR.NETL.DOE.GOV

Andrew Gellman
NETL-RUA Consortium Area Lead
Carnegie Mellon University
(412) 386-5219
Andrew.Gellman@CONTR.NETL.DOE.GOV

Brian Gleeson
NETL-RUA Consortium Area Lead
University of Pittsburgh
(412) 648-1185
Brian.Gleeson@CONTR.NETL.DOE.GOV

Dan Haworth
NETL-RUA Consortium Area Lead
Pennsylvania State University
(814) 863-6269
dch12@engr.psu.edu

Roe-Hoan Yoon
NETL-RUA Consortium Area Lead
Virginia Polytechnic and State University
(540) 231-7056
ryoon@vt.edu

For additional information see the Department of Energy (DOE) National Energy Technology Laboratory (NETL)

http://www.netl.doe.gov/

U.S. Department of Energy

National Energy Technology Laboratory

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

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

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