NETL-RUA
Regional University Alliance

E NEWS

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Shared Intellect • Shared Laboratories • Shared Resources

Featured Partner:

Carnegie Mellon University's Department of Civil and Environmental Engineering (CEE)

Since 2010, the Department of Civil and Environmental Engineering (CEE) at Carnegie Mellon University (CMU) and the National Energy Technology Laboratory (NETL) have enjoyed a fruitful partnership under the umbrella of the NETL Regional University Alliance (NETL-RUA). Although CMU researchers and those at other Alliance universities have worked with NETL scientists for decades, the formation of the NETL-RUA heralded a new era of productive collaborative research between NETL and the university, and CEE researchers have played a key role in the partnership. Currently, CEE has seven faculty and nine PhD students supporting NETL-RUA efforts.

Athanasios Karamalidis

Assistant Research Professor **Athanasios Karamalidis** worked at NETL as an ORISE (Oak Ridge Institute for Science and Education) post-doctoral researcher prior to joining the CEE faculty in 2010. Karamalidis's NETL-RUA work focuses on the impact of geologic carbon dioxide (CO_2) sequestration on groundwater and the geochemistry of shale gas development sites. He has developed a small-scale flow-through reactor system for the investigation of mineral dissolution kinetics when contacted with CO_2-saturated brines under geologic sequestration conditions. His system will be also used for studying the dissolution of various minerals in an international interlab study, where NETL along with more than 22 national and academic partners around the world participate. Among other projects, his recent research explores the potential use of rare earth elements as naturally occurring tracers of fluid migration and indicators of water-rock interactions for shale gas development sites.

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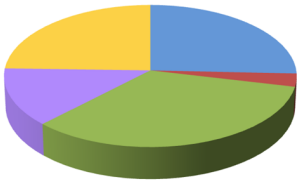
NETL-RUA
Metrics Snapshot

PRODUCTS			
	FY2011	FY2012	FY2013
Publications	194	195	50
Patents Issued	11	12	4
Licenses	9	4	0
Students Graduated	20 PhD	23 PhD	8 PhD
	8 MS	19 MS	1 MS

Product data is updated quarterly.

RESEARCH PERSONNEL



Total = 607

- Graduate Students - 156
- Undergraduate Students - 18
- University Researchers - 204
- URS Researchers - 80
- NETL Researchers - 149

E News is your monthly source for the latest information about NETL-RUA's research, activities, and other important news. If you have information that you would like to feature in future newsletters, send that information to

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Mitchell Small

David Nakles

Gregory Lowry

Kelvin Gregory

Craig Maloney

David Dzombak

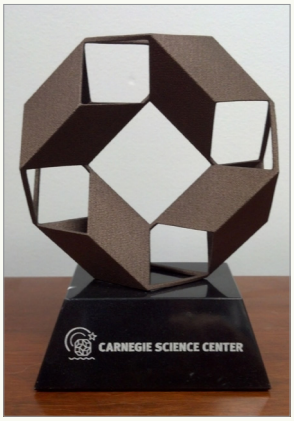
Supporting the National Risk Assessment Partnership, CEE professors **Mitchell Small** and **David Nakles** are working with NETL to demonstrate the application of an integrated assessment model supported by second-generation reduced order models to a real-world CO_2 storage scenario identified within one of the Phase III demonstration test sites of the Regional Carbon Sequestration Partnerships.

CEE professors **Gregory Lowry** and **Kelvin Gregory** are working with NETL to determine the effects of supercritical CO_2 on microbial communities under carbon storage conditions in deep brine aquifers and enhanced oil recovery scenarios. **Djuna Gulliver**, a graduate student supporting this project, is an NETL employee in the Environmental Science Division of the Office of Research and Development (ORD). Professor Gregory is also working with NETL and natural gas producers to gain understanding of how produced water management strategies may be tailored for optimizing the economic and environmental sustainability of oil and natural gas extraction.

The April 2010 Macondo Prospect oil well blowout and the resulting spill in the Gulf of Mexico have demonstrated the importance of foamed cement stability in the safe construction of offshore wells. It is well known that elevated pressures in the wellbore environment have a profound effect on foamed cement properties. CEE Associate Professor **Craig Maloney** and his team are modeling the foamed slurry under conditions that simulate both placement in the well and post placement evolution. **Eilis Rosenbaum**, an NETL researcher and graduate student in CEE, will perform the modeling work.

CEE members have enjoyed numerous recent successes, with several NETL-RUA affiliates receiving awards and appointments. Among those honored was Professor **Dave Dzombak**, recently named Water Environment Federation Fellow for his exceptional accomplishments in the field of water quality. Dzombak, also the newly named department head of CEE, served as a principal investigator with **Dave Nakles** on an NETL-RUA project focused on understanding CO_2-hydrogen sulfide (H_2S)/cement interactions and how they impact the seal integrity of the wellbore with respect to the long-term storage of CO_2 and CO_2-H_2S. Professors **Kelvin Gregory** and **Craig Maloney** each received National Science Foundation grants for work in their respective fields. Gregory's project is "Augmented Surface Acoustic Wave Devices for Microbial Cell Separation Based on Physiological Properties." Maloney's project, "A Data-Driven Statistical Approach to Aging and Elasticity in Colloidal Glasses," will study the fundamental aging of glassy materials from a statistical and microscopic point of view. **Mitchell Small** was appointed to chair a new National Research Council study on Risk Management and Governance Issues in Shale Gas Extraction. CEE and NETL-RUA graduate students **Aniela Burant,** advised by professors Karamalidis and Lowry, and **Hariprasad Parthasarathy,** advised by professors Karamalidis and Dzombak, are supporting NETL-RUA research projects. Each received awards and fellowships for outstanding accomplishment and academic performance. **Arvind Murali Mohan**, another CEE and NETL-RUA graduate student advised by Dr. Gregory, received the best paper award from the Water Environment Federation.

Through opportunities created by the NETL-RUA collaboration, research in CEE at CMU and NETL is advancing national goals of energy security through improvements in the economic and environmental sustainability of natural resources development, according to Dr. Karamalidis, who characterized the environment as "flexible and strongly oriented toward interdisciplinary collaboration."



The Carnegie Science Award trophy is a 3-D printed polyhedron inspired by the Carnegie Science Center logo and was precision-printed by The ExOne Company using a printer designed to create metal products.

NETL-RUA received three Carnegie Science Awards honoring innovation in science and technology on May 3, 2013, at the Carnegie Music Hall in Pittsburgh. Accepting on behalf of the NETL-RUA for Advanced Materials and Corporate Innovation were Cynthia Powell, Director, NETL ORD (left) and Julianne Klara, NETL-RUA Manager (right). Robert Enick, Bayer Professor, Department of Chemical and Petroleum Engineering at the University of Pittsburgh (Pitt), accepted an Environmental award for his Department of Energy-sponsored research.

Fracking Water Quality Parameters Analyzed

The exponential increase in fossil energy production from Devonian-age shales in the northeastern United States, including the Marcellus shale in Pennsylvania and adjoining states, has brought water management questions to the forefront. However, answers to those questions depend on the limited availability of critical water quality parameters for wastewater produced from shale gas wells.

Radisav Vidic

NETL-RUA researcher and Pitt William Kepler Whiteford Professor, **Radisav Vidic**, has been at the forefront of water quality research pertaining to gas well wastewater and is currently performing research as a member of NETL-RUA's Unconventional Resources team. Vidic serves as the Chairman of the Department of Civil and Environmental Engineering in the Swanson School of Engineering at the university.

Vidic, along with fellow Pitt team members **Elise Barbot** (lead author) and **Natasa S. Vidic** and CMU's **Kelvin B. Gregory**, analyzed produced waters from hydraulic fracturing sites in the Marcellus Shale formation, as reported in "Spatial and Temporal Correlation of Water Quality Parameters of Produced Waters from Devonian-Age Shale following Hydraulic Fracturing," in the March 19, 2013 issue of ***Environmental Science & Technology*** (Vol. 47, issue 6).

Hydraulic fracturing, which is needed to recover natural gas from unconventional sources, involves pumping millions of gallons of water into the subsurface. A significant amount of water containing extremely high concentrations of dissolved solids is recovered at the surface, together with the natural gas. Understanding the source, composition, and distribution of these components is the first step for developing sustainable water management approaches.

This study of waters produced from 160 such wells may help guide water management strategies for development of unconventional gas resources. Chloride was used as a reference for the comparison, as its concentration in produced water varies with time of contact with the shale. Most major positive ions, or cations (e.g., calcium, magnesium, strontium), were well correlated with chloride concentration, while barium concentration was strongly influenced by geographic location, with higher levels in the northeastern than in the southwestern areas of the region.

Major cations did exhibit variations that cannot be explained by simple dilution of existing formation brine with fracturing fluid, especially during the early flowback water production when the composition of the fracturing fluid and solid-liquid interactions influence the quality of the produced water.

Noteworthy Achievements

Xueyan Song

Assistant Professor **Xueyan Song** of West Virginia University's (WVU) Department of Mechanical and Aerospace Engineering recently earned a Faculty Early Career Development award from the National Science Foundation (NSF) to investigate ways to improve the sustainability of our energy infrastructure through waste heat recovery. With this award, Song plans to explore ways to improve the energy conversion efficiency of thermoelectric oxides, which possess the ability to directly transform temperature differentials into electrical power. The award is funded by the Ceramics Program in the Division of Materials Research at NSF. Dr. Song's NETL-RUA work in support of the Advanced Gasification team focuses on providing scanning electron microscopy/transmission electron microscopy (TEM) analyses in the areas of refractory development and ash management for improving performance and service life of existing gasifier liner materials. As part of the NETL-RUA Fuel Cell team, Professor Song employs TEM to identify the nano-scale features that appear in fuel cell electrodes under various operating conditions that in turn provide insight into mechanisms of cell degradation and methods of improving cell performance.

Jeen-Shang Lin

Jeen-Shang Lin, associate professor of civil and environmental engineering at Pitt's Swanson School of Engineering, was recently elected a Fellow of the American Society of Civil Engineers (ASCE). It is a prestigious honor held by fewer than five percent of ASCE members. ASCE Fellows are recognized for distinguished careers that have contributed significantly to the Civil Engineering profession. Lin's research focuses on the mechanics and modeling of rock drilling for energy production. Supporting the Unconventional Resources team, Lin's NETL-RUA projects provide hydrate-relevant, experimentally measured key physical properties and models that may be incorporated into coupled geomechanical analysis for predicting the behavior of hydrate-bearing sediments.

Congratulations to WVU graduate student **Xiaoke Chen**, who successfully defended her dissertation entitled "Aging Effects of the Cathode and Determination of Single Electrode Performance in a Solid Oxide Fuel Cell" to earn a Ph.D. in Chemistry. Chen's NETL-RUA work under WVU professor Harry Finklea supported the Fuel Cells team and focused on the investigation, deconvolution, and assessment of the contribution of specific processes to the performance of solid oxide fuel cell electrodes.

Technology Spotlight

Database to Aid Advanced Alloy Processing

Paul Jablonski of the Process Development Division in ORD at NETL and Professor **Zi-Kui Liu**[1] of the Materials Science and Engineering department at the Pennsylvania State University are developing a new CALPHAD (calculation of phase diagram) modeling thermodynamic database to aid in slag formulation for electro-slag remelting (ESR). The first version is now complete and includes the elements aluminum, calcium, chromium, fluorine, iron, magnesium, manganese, nickel, oxygen, silicon and titanium. Assessed systems include binary, ternary, and oxide systems.

ESR Process

ESR is a manufacturing process employed in the production of advanced high-temperature steels and nickel superalloys for mission-critical applications including thermal power stations, nuclear power plants, aircraft, and military technologies. The process is used to refine and purify the chemistry of alloy ingots and is a critical step in the production of high-performance alloys.

The new Vacuum Arc Remelting/ESR unit installed in the NETL Albany Melt Lab

The slag plays a critical role in the ESR process, which uses an as-cast vacuum induction melted alloy ingot as a consumable electrode. An electric current is passed through the electrode and into an engineered slag, which gradually melts the tip of the electrode. As the electrode melts, drops of molten metal descend through the slag to the mold, where they slowly freeze to form the new ESR ingot from the bottom up. Impurities are cleaned from the molten alloy by chemically reacting with the slag and/or floating with it to the top. The resultant ESR ingot is of the high chemical purity necessary for mission-critical components.

A better understanding of the slag is needed in order to produce the desired ingot chemistry (especially with regard to trace elements, which can be either detrimental or beneficial) and ingot structure. This understanding and control of the slag has the potential to provide higher-quality ESR melted materials, which will be at the core of the fossil energy power plants of the future such as advanced-ultrasupercritical (A-USC) coal-fired steam plants.

The new database provides the foundation for NETL-RUA work on alloys, slag chemistries, and alloy-slag interactions. The next step in the development of the database is to establish and incorporate slag physical properties such as thermal and electrical conductivities, density, viscosity, and variations in temperature and chemistry. NETL-RUA researchers plan to utilize this database to optimize the re-melt processing of steam turbine rotor alloys for A-USC plants.

[1] Professor Liu's NETL-RUA efforts support the NETL Innovative Process Technologies team and focus on the first-principles calculations based on density functional theory and the CALPHAD (Computer Coupling of Phase Diagrams and Thermochemistry) modeling of binary and ternary alloy.

Upcoming Events

- **American Association of Petroleum Geologists Annual Convention & Exhibition**
  May 19–22, 2013
  David L. Lawrence Convention Center, Pittsburgh, PA
- **Grid Technologies Collaborative Meeting**
  June 9, 2013 – *Reception* & June 10, 2013 – *Meeting*
  Arlington, Virginia

  For details: http://www.cpe.vt.edu/gtc/

Your favorite issues of the NETL-RUA E NEWS are now available on the MOSS and the NETL-RUA website (www.netl.doe.gov/rua)

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