NETL-RUA
Regional University Alliance

E NEWS

Shared Intellect • Shared Laboratories • Shared Resources

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CCSI Releases Computational Tools and Models Ahead of Schedule

The Carbon Capture Simulation Initiative (CCSI) successfully pre-released its first set of computational tools and models as the CCSI Toolset at the October 2012 Industry Advisory Board (IAB) meeting in San Francisco, California, one year ahead of schedule. This release is the result of intense industry interest in getting early access to the tools as well as the phenomenal progress of the CCSI technical team.

The 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 reduced-order models (ROMs) from reacting multiphase flow simulations and running thousands of concurrent process simulations for optimization and uncertainty quantification. These initial components provide new models and computational capabilities that will accelerate the commercial development

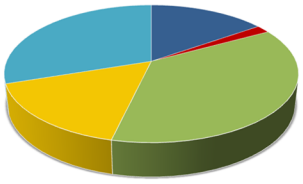
>> See **CCSI**, *Page 2*

NETL-RUA
METRICS SNAPSHOT

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

Product data is updated quarterly.

RESEARCH PERSONNEL



Total = 494

- **Graduate Students - 75**
- **Undergraduate Students - 9**
- **University Researchers - 181**
- **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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What's in This Issue

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>> **CCSI**, *Continued from Page 1*

of carbon capture technologies as well as a broad range of technology development in general (power, refining, chemicals production, gas production, etc.).

Ordinarily, new technology development from concept to commercialization takes 20 to 30 years. The CCSI toolset will enable industry to reduce the time, risk, and expense of new development—from discovery through demonstration to widespread deployment—to one-third of the time typically required.

The aerospace and automotive industries have shown that simulations can be used effectively to accelerate technology development. CCSI will combine recent advances in simulation technology to develop a science-based capability to assess and mitigate the risk of scaling up carbon capture technologies and reduce development costs and time.

The project targets post-combustion carbon capture, which is expected to have the greatest immediate impact on U.S. pulverized coal power plants that are currently generating nearly 40 percent of the nation's electricity and expected to emit 95 percent of the carbon dioxide from United States coal-based power plants between 2010 and 2030.

CCSI comprises a team of five DOE national laboratories (NETL, Lawrence Berkeley, Lawrence Livermore, Los Alamos, and Pacific Northwest), three NETL-RUA universities (Carnegie Mellon University, the University of Pittsburgh and West Virginia University), Princeton University, Boston University, The University of Utah, and URS. This team also includes the active participation of the IAB, comprising nearly 20 industry partners charged with guiding CCSI researchers in the development of a toolset which industry can use when moving from concept to commercialization. "Because carbon capture systems are not yet required at any of the 600-plus plants across the country, CCSI works closely with industry to make the tools easier to adapt to existing design technologies. These tools will make it easier for utility companies to meet such requirements if and when they are enacted, and could help companies doing business in countries where controls are already in place," said Madhava Syamlal (NETL), CCSI Project Director. The total cost savings that could be realized by using the CCSI toolset to scale up and widely deploy just one carbon capture technology is estimated at approximately $500 million.

NETL Joins Commercialization Alliance to Accelerate Tech Transfer

In 2011, a Presidential Memorandum was issued stipulating that federal research laboratories develop plans to establish performance goals to increase the number and pace of effective technology transfer and commercialization activities.

To meet the stipulations of the memorandum, NETL has engaged the services of *Innovation Works*, a technology commercialization organization headquartered in Pittsburgh, Pennsylvania, to lead a consortium of partners known collectively as the Commercialization Alliance. Other consortium partners include INNOVA Commercialization Group, Oregon BEST (Oregon Built Environment & Sustainable Technologies Center), and MATRIC (Mid-Atlantic Technology Research & Innovation Center). These partners will rely on input and support from the NETL-RUA, as well as from TechConnect WV and the Energy Alliance of Greater Pittsburgh, to achieve three specific objectives: (1) increase the number of NETL technologies evaluated for commercialization, (2) increase the number of NETL licenses, and (3) increase the number of newly formed businesses. The Commercialization Alliance will employ Innovation Works's proven agile innovation commercialization process, which will be applied to the development of technologies from pre-concept through market entrance, and aims to establish a new commercialization culture within NETL. Institution of this process will translate to an increase in licensing revenue as well as increased company formation, industry activity, and job growth in the participating regions of Pennsylvania, West Virginia, and Oregon. Most importantly, this will enhance NETL-RUA's reputation and place it on the cutting edge of commercialization processes within national research institutions. Ultimately, these achievements will increase NETL-RUA's stature as a commercialization leader among national research institutions.

NETL Hosts Topical Conference at the AIChE Annual Meeting

Despite the threat of Hurricane Sandy, the American Institute of Chemical Engineers (AIChE) 2012 Annual Meeting was held from October 28 through November 2 and touted record-breaking attendance. Pittsburgh welcomed over 6,000 attendees to the meeting, which was held at the David L. Lawrence Convention Center and highlighted the role of clean energy technologies in developing a strong economy and improving quality of life.

NETL hosted one of the featured topical conferences, comprising 22 of the meeting's more than 800 technical sessions, on ***Accelerating Fossil Energy Technology Development through Integrated Computation and Experimentation***. NETL-RUA members were integral to the success of these sessions as representatives from NETL, URS, and all five NETL-RUA member universities contributed presentations or chaired sessions. Selected presentations will be published in a dedicated issue of the journal ***Energy and Fuels***.

These sessions addressed a multitude of topics, including:

- Advanced gasification concepts to reduce the cost of electricity while maintaining the highest environmental standards
- Controlling emissions of mercury and other trace elements
- Improvements in commercial processes for producing hydrogen
- Membranes, solvents, and sorbents for gas separation
- Novel approaches to utilizing carbon dioxide
- Modeling the behavior of carbon dioxide injected into geologic formations
- Methods to evaluate the cost and performance of carbon capture, utilization, and storage technologies

As regional media coverage emphasized, Pittsburgh is a desired destination for many technical organizations, as the city mirrors many of the key interests of their constituents. Those interests include an economy driven by innovation, plentiful research and development opportunities, and a regional commitment to advancing energy solutions across a diversified portfolio of energy resources. "My sense is that industry is drawn to this region because of the assets we offer," observed NETL Director Anthony Cugini. "We're home to chemical industry leaders with a long history of successful innovation. We have a well-trained workforce and business development organizations keenly interested in the energy economy. We are sharply focused on sustainable energy use, and we are a national leader in sustainable building design and operation."

Chuck McConnell, DOE Assistant Secretary for Fossil Energy, provided a well-received keynote address on harnessing scientific development and business principles to achieve fossil energy sustainability. Both Assistant Secretary McConnell and Dr. Cugini have roots in chemical engineering at NETL-RUA member universities, having received degrees in the field from Carnegie Mellon University and the University of Pittsburgh, respectively.

The 2013 AIChE Annual Meeting will be held in San Francisco, California from November 3 through November 8. For more information visit the AIChE website: http://www.aiche.org/conferences/aiche-annual-meeting/2013.

Upcoming Events

- **NETL-RUA Spring Meeting** (details in February issue)
  Tuesday, March 5, 2013
  Waterfront Place Hotel, Morgantown, WV
- **PITTCON™ Conference & Expo**
  March 17–21, 2013
  Pennsylvania Convention Center, Philadelphia, PA
- **12th Annual Conference on Carbon Capture & Sequestration**
  May 14-16, 2013
  David L. Lawrence Convention Center, Pittsburgh, PA
- **American Association of Petroleum Geologists (AAPG) Annual Convention & Exhibition**
  May 19–22, 2013
  David L. Lawrence Convention Center, Pittsburgh, PA

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Technology Spotlight

WVU's Liu Studies Keys to Corrosion Resistance

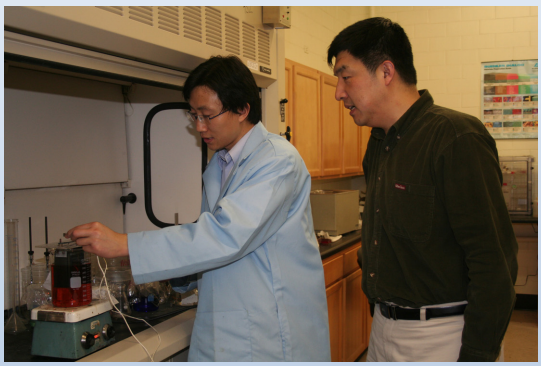
In the early 20th century, a type of metalworking known as peening—striking the surface of a metal with a hammer or metal, glass, or ceramic shot— was discovered to decrease metal fatigue. By the 1950s, peening was an accepted practice for increasing the surface compressive strength of a metal and decreasing its surface tensile strength, thereby reducing crack formation. However, the effect of hammer peening on the corrosion resistance of metal alloys has not been widely investigated nor fully understood, according to West Virginia University Associate Professor Xingbo Liu who has been investigating the topic.

In the early 21st century, growing worldwide demand for oil makes understanding the effects of hammer peening on alloys especially important in deep-sea oil production. Oil-grade alloy 718, a superalloy used by the oil industry for casings and piping, particularly interests Liu and his colleagues. The metal must be able to withstand the extreme pressures, temperatures, and corrosive salts in deep-sea environments. Even before the 2010 Macondo oil spill, engineers were concerned about the potential failure of metal casings and piping. For example, the 2006 Prudhoe Bay spill stemmed from a dime-sized hole in the transit pipeline caused by corrosion.

Liu received funding through the NETL-RUA to conduct experiments and simulations to characterize and evaluate the corrosion of superalloy 718 samples that had been hammer-peened and passivated. Passivation uses heat aging to create a thin coating of oxide on the metal's surface to combat corrosion. Liu's project addressed key metal-based failures by examining the results of corrosion experiments on drilling, completion, and production piping.

Last fall, Liu and his NETL and Baker Hughes, Inc. colleagues presented their research at the 12th International Symposium on Superalloys.† The event is held every four years by The Minerals, Metals & Materials Society to share the latest technical information about high-strength, high-temperature alloys.

They reported that compressive residual stresses introduced by hammer peening significantly increased the corrosion resistance of oil-grade alloy 718 in a 3.5 weight percent sodium chloride solution used to mimic seawater at room temperature. Also, passivating the alloy with a thin layer of gamma-prime/gamma-double-prime (γ′/γ″) phases of a chromium-enriched oxide film close to the top of the surface of the alloy improved corrosion resistance.



Former graduate research assistant Junwei Wu and his advisor, WVU Associate Professor Xingbo Liu, investigated corrosion-resistant fuel cell interconnects.

The project is one of several materials-related investigations that Liu has conducted through the NETL-RUA and its predecessor, the NETL Institute for Advanced Energy Studies (NETL-IAES). He credits such collaborations with allowing him to become a nationally recognized and competitive researcher, citing the 2011 ***R&D*** 100 Award he received as part of a team that included NETL's Randall Gemmen and Chris Johnson for their work on corrosion-resistant fuel cell interconnects. These collaborations enable him to discover the fundamentals behind existing technologies, such as peening, and develop new technologies for the environmentally sensitive use of fossil fuels.

† EFFECTS OF HAMMER PEENING AND AGING TREATMENT ON MICROSTRUCTURE, MECHANICAL PROPERTIES AND CORROSION RESISTANCE OF OIL-GRADE ALLOY 718; Ting Chen[1], Hendrik John[2], Jing Xu[2], Jeffrey Hawk[3], Xingbo Liu[1];

[1] Mechanical & Aerospace Engineering Department, West Virginia University, Morgantown, WV 26506;

[2] Baker Hughes Incorporated, Celle 29221, Germany;

[3] National Energy Technology Laboratory, Albany, OR 97321-2198