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Regional University Alliance

NEWS

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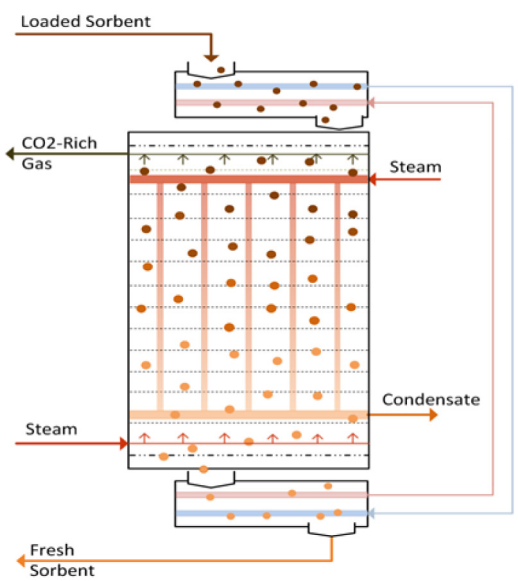
January 2014
VOLUME 4, ISSUE 1

The Tools of the Trade: NETL-RUA Helps CCSI Nurture Innovations in Carbon Capture

Imagine you own a factory that produces coolers. You have an idea for a new cooler that doesn't leak, can't be crushed, and never becomes discolored or mildewed. Now, imagine that a suite of modeling and simulation tools could help you design your improved cooler faster, identify any of the design's flaws, and get the coolers into stores sooner—and for less money—than you expected. The Carbon Capture Simulation Initiative (CCSI), led by the National Energy Technology Laboratory (NETL), has done just that. Only, instead of helping to devise new ways to keep drinks cold, CCSI's tools help bring to market technologies that keep carbon dioxide (CO_2) from warming up our world.



Schematic of a dynamic/steady-state moving bed reactor model for regenerating a solid sorbent for carbon capture

Funded through the Office of Fossil Energy, CCSI seeks to hasten the commercialization of carbon capture technologies. University researchers—including researchers from Carnegie Mellon (CMU) and West Virginia Universities (WVU), both NETL-Regional University Alliance (NETL-RUA) member organizations—collaborate with researchers at NETL's Office of Research and Development (ORD) to further CCSI's mission. CCSI's software, called the CCSI Toolset, contains tools and models that lend credence to carbon capture designs that are advantageous. It also makes it easier to distinguish favorable concepts from unfavorable ones, shortens the time it takes to design and troubleshoot a new device or process, and more accurately represents the risk associated with scaling up a technology. The Toolset was originally released in September 2012, and CCSI released a new, expanded version in October 2013.

"Responding to industry feedback, the latest release enables users to more effectively utilize advanced computational capabilities to accelerate technology development," says CCSI Technical

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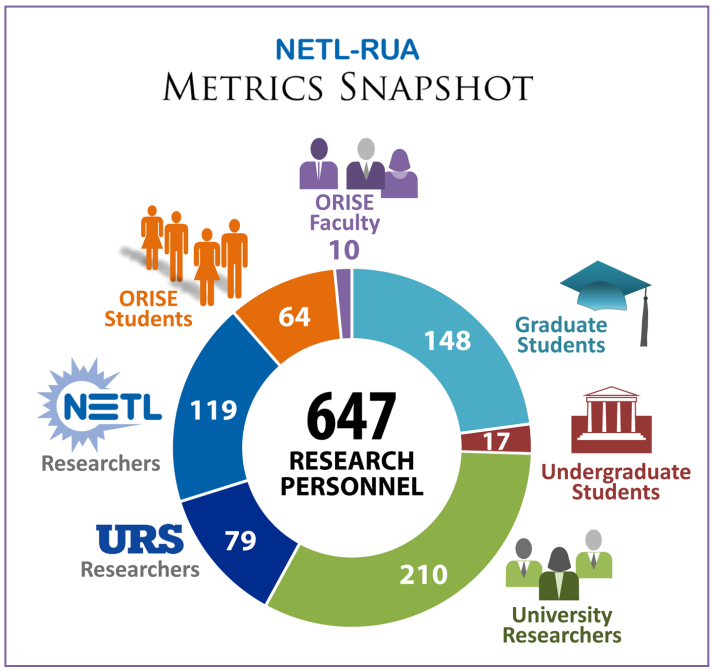
What's in This Issue

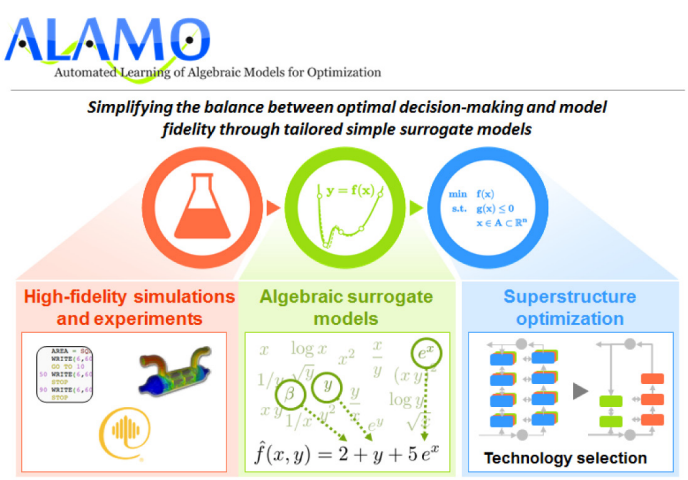
Contact:
Julianne Klara
julianne.klara@netl.doe.gov
412-386-6089



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

Team Lead **David Miller**. "We are working closely with several companies who have licensed the Toolset to ensure it is successfully deployed and utilized within their organizations." Five companies—General Electric, Alstom, Phillips66, Babcock & Wilcox, and Chevron—now license the Toolset.

The latest version of the Toolset includes an integrated Framework for Optimization and Quantification of Uncertainty and Sensitivity (called "FOQUS"), which makes it possible to run hundreds of simulations in parallel. It also includes an algebraic surrogate model builder called "ALAMO" (developed at CMU) that is far faster than its predecessor, a new computational fluid dynamics model to predict particle attrition, tools for statistics-based model validation, a new technical risk model, and an updated financial risk model. These updates (and the many others included in this release) may help produce the next big technology in carbon capture.



This figure highlights the major functionality of ALAMO, a code developed at CMU for the automated learning of algebraic models for optimization. ALAMO can take data from high-fidelity simulations or experiments and convert them to a simpler algebraic format, which can then be used to optimize complete processes.

Digging for Data: geoWELL Helps NETL-RUA Researchers Mine the Web for Information

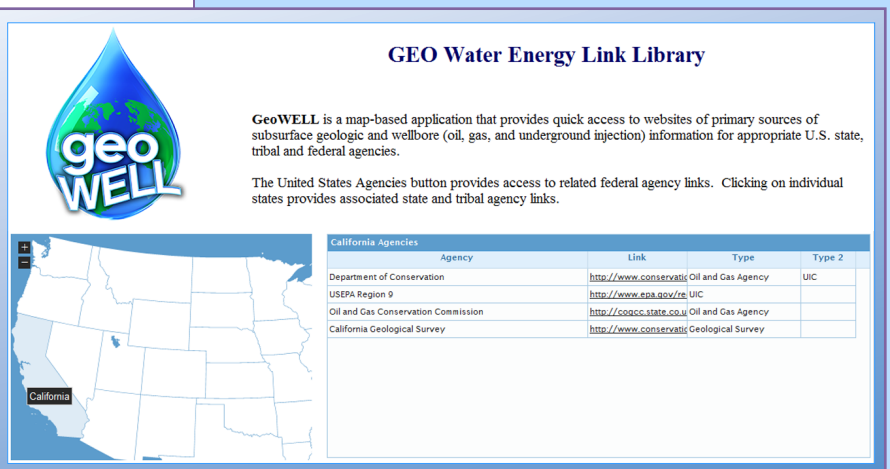
Since its launch in the spring of 2013, geoWELL (or "geo-Water Energy Link Library") has been helping researchers access subsurface-geologic and wellbore information. "It was built to support NETL researchers so they can quickly find the primary source for key information on subsurface data, such as wellbore permits . . . [and] underground injection data," explains **Kelly Rose**, an NETL research geologist, "but we made it public to support this same need by other groups." NETL researchers, along with Sextant Technical Services, the Groundwater Protection Council, Coordinate Solutions, and URS Corporation (an NETL-RUA member organization) created the site.

Clicking a state on geoWELL's interactive map directs researchers to webpages run by the state's agencies, such as its geological survey or department of natural resources. So, by clicking California, a researcher can view geologic maps of the state or learn whether a particular injection well is in operation. What's more, geoWELL provides links to websites associated with federal and tribal agencies. "Instead of having to go to multiple resources, or doing a Google search where you get thousands of returns, this is one place to look at all the data sets," says Sextant Technical Services' **Chad Rowan**.

And unlike the results of a Google search, all of the information geoWELL provides is accurate. Relying on secondary data sources—rather than the primary sources geoWELL links to—can hamstring a research project.

geoWELL is part of the Energy Data eXchange (EDX), an online system that NETL's ORD maintains to give NETL-affiliated researchers access to reliable, relevant energy data. geoWELL is especially pertinent to NETL's Carbon Storage Program, which the NETL-RUA Carbon Storage research team supports. As Rowan, the daily operations lead for EDX, says, geoWELL is a "one-stop shop for energy resources."

geoWELL makes it easy for researchers investigating subsurface geology or wellbores to find reliable primary sources. Clicking a state on geoWELL's interactive map brings up a list of related links.



Technology Spotlight

NETL-RUA Researchers Pursue the Advantages of Chemical Looping Combustion

Chemical looping reactors are an exciting new technology for industrial steam production--a technology that NETL-RUA researchers are working to advance.

Chemical looping combustion (CLC) differs from conventional combustion in that air and fuel never come into direct contact with each other. Instead, oxygen is delivered to the fuel in the form of oxygen carriers such as iron oxide, copper oxide, or other solid materials. The advantage of this system is the resulting flue gas consists purely of CO_2 and water. Therefore, CO_2 can be isolated for storage or conversion to other products by simply condensing the water, a straightforward and relatively inexpensive process for capturing CO_2.

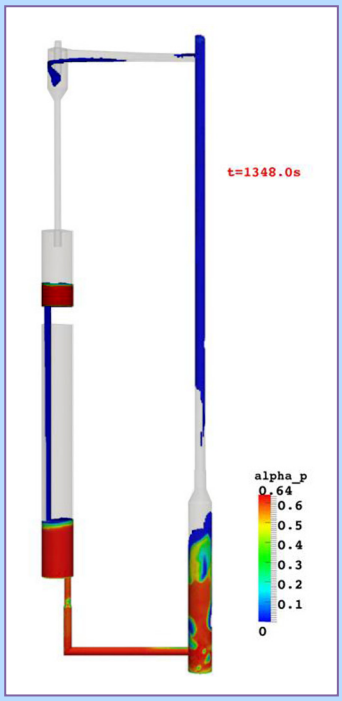
CLC shows great promise as an innovative, environmentally friendly way to use fossil energy fuels to produce steam—or, perhaps, to generate power for other applications one day. It is not without drawbacks, however. For instance, oxygen carriers may not be as durable as they need to be, or operational issues may limit the number of suitable oxygen carriers. "It will be difficult to attract private-sector funding from financial institutions because there are a lot of technical issues that still need to be addressed," says **Doug Straub**, a mechanical engineer at NETL who is one of the leaders of the CLC task. "No bank will provide a loan to build a CLC plant until they have more confidence that a profit can be realized."

Researcher James Fisher, of URS Corporation works at NETL's single bed fluid reactor, which provides data that are relevant to NETL's chemical looping reactor.

To increase investor confidence, NETL-RUA scientists are conducting research to overcome the technical issues that remain. The effort is part of the NETL-RUA Industrial Carbon Management Initiative and is made possible by American Recovery and Reinvestment Act funding. It aligns with the Office of Fossil Energy's mission to keep traditional energy sources secure and affordable, while enhancing environmental protection. NETL-RUA researchers have pursued several research projects as part of the initiative. For example, **David Greve**, an electrical engineering professor at CMU, has worked to develop a sensor that can measure flow rates of oxygen carriers at temperatures ranging from 800 to 1,000 degrees Celsius. **Götz Veser**, a professor in the University of Pittsburgh's (Pitt) Catalytic Reaction Engineering Group, has done research to synthesize and evaluate nanostructured oxygen carriers. And **John Kitchin**, an associate professor of chemical engineering at CMU, has run numerical simulations of oxide materials to identify new oxygen carriers and improve existing ones.

"NETL is the first to initiate a coordinated effort of [chemical looping] research that incorporates experimental testing, [computational fluid dynamics (CFDs)] simulation, and techno-economic studies to accelerate technology development," says **Steve Carpenter**, a chemical engineer with URS Corporation. If the research team's efforts pay off, new ways for industries to cleanly produce steam could start bubbling up.

Modeling and simulation technologies are integral to exploring how a chemical looping system performs. NETL-RUA researchers use four CFD codes for this purpose: Multiphase Flow with Interphase eXchanges (MFIX), OpenFOAM, Barracuda, and Fluent. Tools such as these have enabled NETL-RUA researchers to view fluctuating concentrations of solids in different parts of a chemical looping reactor and use this information to reduce how often reactor filters need to be emptied.



Right: A simulation shows the changing concentrations of solids in different parts of a chemical looping reactor during operation. As the percentage of solids increases in a given area, the colors depicting the percentages change from blue to green, yellow, orange, and (if the percentage reaches 64 percent) red.

An Important Charge: NETL-RUA Works to Ensure the Safety of Hydraulic Fracturing

Washington County, Pennsylvania, is home to the Pennsylvania Trolley Museum and an annual covered-bridge festival. It's also home to a test site that helps researchers keep track of the effects hydraulic fracturing can have on the environment.

The shale-gas industry gave NETL access to the Washington County site, which overlies the Marcellus Shale Formation, so that NETL could evaluate how preparing a site for a well pad, drilling and completing the wells, and putting them into operation can change environmental conditions. Recently, NETL researchers **Garret Veloski**, **Jim Sams**, and **Rod Diehl** conducted electromagnetic surveys at the Washington County site and discovered that the background conductivity across the well pad area there is low. In other words, the rain-leached soil in the well pad area could not pass much electrical current. This is good news for researchers. "Water produced from oil and gas wells is saline and highly conductive because it is brine (evaporated seawater) from the formation," says **Richard Hammack**, a physical scientist at NETL. "[P]roduced-water leaks should be easily detected and mapped with [electromagnetic] methods, especially in areas where the baseline soil conductivity is low."

This work supports ORD's efforts to fulfill NETL's obligations under the Energy Policy Act of 2005, which involves investigating the environmental impacts of oil and natural gas development, among other topics.[1] Researchers from CMU, Pitt, the Pennsylvania State University, and WVU—all NETL-RUA member organizations—have been involved in the research taking place at the Washington County site. Their efforts support NETL-RUA's Unconventional Energy Resources Initiative, and they will help minimize the impact of hydraulic fracturing on the environment as the industry grows in Washington County and other areas as well.

[1] Department of Energy, *Energy Policy Act of 2005 (Ultra-deepwater and Unconventional Resources Program)*, n.d., http://www.netl.doe.gov/technologies/oil-gas/EPAct2005/NETL_CompRD.html, accessed December 20, 2013.

To conduct electromagnetic surveys of the Washington County site, NETL researchers first divided the site into multiple parallel lines. They then walked or drove over those lines with a multi-frequency electromagnetic instrument. The resulting electromagnetic data could reveal the distribution of conductivity at different depths.

NETL-RUA's work in support of the Energy Policy Act of 2005 wasn't limited to the electromagnetic surveys at the Washington County site. Researchers reviewed new data sets generated through the Environmental Defense Fund air monitoring field project, and identified new values for unconventional well emission completions for use in calculating new emissions factors. They also ground-truthed legacy well surveys at the Washington County site. This task involved investigating 17 sites in the field that (according to helicopter-based magnetometer measurements) could have been well sites, confirming the inclusion of 13 wells in the Pennsylvania Internet Record Imaging System (PA*IRIS), and spotting location errors in PA*IRIS.

UPCOMING EVENT

NETL-RUA Spring Meeting | March 11, 2014 | Waterfront Place Hotel | Morgantown, WV

For more information and to register, please visit: http://netldev.netl.doe.gov/events/2014-netl-rua-spring-meeting.

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