

NETL-RUA Engineer Earns Presidential Award

On July 23, 2012, President Obama named 96 researchers as recipients of the Presidential Early Career Awards for Scientists and Engineers (PECASE), the highest honor bestowed by the United States Government on science and engineering professionals in the early stages of their independent research careers.

One of our own, Dr. John Kitchin, was among those honored. Kitchin has been recognized for his NETL-RUA research in electrochemical separations for energy applications, which has the potential to enable clean coal technologies that meet U.S. Department of Energy (DOE) goals for carbon capture, and his dedication to educating the next generation of scientific leaders.



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

Dr. Kitchin was nominated for the award by DOE's Office of Fossil Energy for research efforts such as his "Ion Exchange Resins as Carbon Dioxide (CO₂) Sorbents for Post-combustion CO₂ Capture" project, which he performs as part of NETL-RUA. In his nominating letter, Assistant Secretary for

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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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NETL-RUA METRICS SNAPSHOT

PRODUCTS		
	FY2011	FY2012
Publications	194	70
Patents	11	2
Licenses	9	4
Students Graduated	20 PhD	23 PhD
	8 MS	18 MS

RESEARCH PERSONNEL



Total = 521

- Graduate Students - 102
- Undergraduate Students - 12
- University Researchers - 181
- URS Researchers - 83
- NETL Researchers - 143

Product data is updated quarterly.

July/August 2012

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Fossil Energy Charles D. McConnell said about Dr. Kitchin, “Many young scientists benefit from hearing this professor lecture, and all of us benefit from his research, which has focused repeatedly on improving the efficiency of energy processes . . . His rapid ascent to the top of his field is a credit not only to his high standards of scientific rigor, but just as importantly, to his commitment to communicate what he knows through published papers, lectures, and mentoring the young scientists who may follow in his footsteps.”

Dr. Kitchin has made important contributions to the development of carbon capture technology, advancing national efforts to enable the environmentally responsible use of fossil fuels in 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 Dr. Kitchin’s contributions to fundamental advances in the computational modeling and design of new catalyst materials, for which he received a DOE research grant under the 2010 Early Career Research Program.

Dr. Kitchin is an associate professor of chemical engineering at Carnegie Mellon University (CMU). Aside from his research, Kitchin 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, Dr. Kitchin was awarded the *Kun Li Teaching Award* in 2010 for best lecturer in his department, as voted on by the senior class at CMU.

Of this year’s awardees, President Obama said “Discoveries in science and technology not only strengthen our economy, they inspire us as a people...The impressive accomplishments of today’s awardees so early in their careers promise even greater advances in the years ahead.”

The awards, established by President Clinton in 1996, are coordinated by the Office of Science and Technology Policy within the Executive Office of the President. Awardees are selected for their pursuit of innovative research at the frontiers of science and technology and their commitment to community service as demonstrated through scientific leadership, public education, or community outreach.

[Click here](#) for a complete listing of this year’s awardees.



NETL-Developed Technology Recognized with R&D 100 Award

An NETL-developed technology, Basic Immobilized Amine Sorbent (BIAS) Process, has been recognized by R&D Magazine as among the 100 most technologically significant products introduced into the commercial marketplace within the past year.

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. Additionally, team members Jessica Sosenko of NETL and Kathryn Klos of URS worked closely with strategic partner ADA Environmental Solutions, Inc. (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.

The BIAS process encompasses a portfolio of techniques for the production of regenerable immobilized amine-based sorbents

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★ **Noteworthy Achievements** ★

Michael Gao, URS, was recognized as a guest editor for *JOM*, the Journal of The Minerals, Metals & Materials Society (TMS), and has completed organizing a special July Issue titled, “Computational Thermodynamic and Kinetic Modeling of High-Entropy Alloys and Amorphous Alloys.” His introductory overview for this issue was published online June 30, 2012.

NETL-RUA team members were awarded 800,000 service units by the Extreme Science and Engineering Discovery Environment (XSEDE) for a joint research proposal titled, “First-Principles Design of Advanced Materials for Clean Coal Research and Extreme Environments.” This award will be a significant help to URS researchers and university partners at NETL-Albany in utilizing external high-performance computing resources to support fossil energy research. The team members include **Michael Gao** (URS), **De Nyago Tafen** (URS), **Mike Widom** (CMU), and **Lizhi Ouyang** (Tennessee State University).

CMU researcher and NETL-RUA graduate student **Robin Chao** successfully defended his PhD dissertation titled, “Improving Solid Oxide Fuel Cell Cathode Performance by Infiltrating Mesoporous Perovskite Coatings” and was approved by committee members Paul Salvador (advisor, CMU), John Kitchin (CMU), Jay Whitacre (CMU), Gregory Rohrer (CMU), and Kirk Gerdes (NETL).

CMU and NETL-RUA researcher **Walter (Rich) Alesi** received his PhD in Chemical Engineering in May and accepted a position working with Intel. Alesi worked under John Kitchin on an NETL-RUA project titled, “Investigation and Mechanistic Study of Amine-Enriched Sorbents for Post-Combustion CO₂ Capture.”

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and provides a methodology for the capture of CO₂ from flue gas streams. Low-cost, regenerable amine-based sorbents offer many advantages over existing technologies including increased CO₂ capture capacity, reduced corrosion, lower energy requirements and costs, and minimized water usage. Additionally, amine-based sorbents are scalable for use in industrial applications, including coal combustion and gasification-based power generating systems.



McMahan (Mac) Gray

Application of this technology is expected to reduce 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.

Additionally, the process can capture CO₂ 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.

R&D 100 Awards are regarded by many within industry, government laboratories, and academia as instrumental in identifying state-of-the-art technologies and helping to move innovative science into the public marketplace. The annual awards, known as the “Oscars of Invention,” are selected by an independent panel of judges and the editors of R&D Magazine.

Energy Secretary Steven Chu congratulated this year’s R&D 100 award winners, saying “The research and development at the DOE’s laboratories continues to help the nation meet our energy challenges, strengthen our national security and improve our economic competitiveness.”

This year’s winners will be recognized at the R&D 100 Awards Banquet on November 1, 2012, at the Renaissance Orlando at Sea World.



NETL’s Annual Multiphase Conference

The NETL annual Multiphase Conference hosted by the Office of Research and Development, Computational Science Division was held from May 22 to May 24 at the National Research Center for Coal and Energy (NRCCE) in Morgantown, West Virginia. The conference brought together 79 researchers across industry and academia from the U.S. and Canada, to discuss their latest research in the area of multiphase flows and application of simulation technology in modeling complex gas-solid flows. There were 38 presentations, including five NETL-RUA projects, covering areas of interest to the multiphase community such as fundamental multiphase model development and the application of computer simulation to gasification, chemical looping and CO₂ adsorption along with application of advance diagnostic tools to gas-solid flows. On the first day, the keynote lecture was provided by Prof. Michel Louge from Cornell University. Prof. Louge discussed the heat transfer enhancement encountered in suspensions of agitated solids. On the second day, the keynote lecture was provided by Dr. Timothy Healy from ExxonMobil Research and Engineering. Dr. Healy discussed the use of filtered two-fluid models for gas-solid flows and their industrial application. NETL-RUA research teams led by Professors Danesh Tafti, Chris Roy and Ranga Pitchumani from Virginia Tech (VT) and Professor Richard Turton from West Virginia University (WVU) presented the latest findings of their respective NETL-RUA projects.



The multiphase conference proceeding is available at <http://www.netl.doe.gov/publications/proceedings/12/mfs/>.

★ *See Technology Spotlight (p. 4) for Pitchumani’s Research* ★

UPCOMING EVENTS

- **Materials Science & Technology 2012 Conference & Exhibition**
October 7–11, 2012 | Pittsburgh, Pennsylvania
- **2012 Pittsburgh Coal Conference**, October 15–18, 2012,
David L. Lawrence Convention Center | Pittsburgh, PA
- **2012 AIChE Annual Meeting, Cleaner Energy, Stronger Economy, Better Living**,
October 28–November 2, 2012, David L. Lawrence Convention Center | Pittsburgh, PA
- **NETL-RUA Fall Meeting: Energy & Innovation Conference**, November 28–29, 2012,
Southpointe Hilton Garden Inn | Canonsburg, PA

Look for more information on these events in upcoming issues of the newsletter

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Online





Technology Spotlight

QUICKER Methodology

Multiphase systems operate in an environment of uncertainty. This uncertainty exists both in the parameters governing the process as well as in the process behavior, and the interactive effects of this uncertainty lead to variability in the system performance and process outcomes. Uncertainty quantification, through stochastic computational modeling and analysis, is an important tool for understanding these effects and for designing systems to be robust in the face of the uncertainties. Conventional methods of uncertainty quantification, such as Latin Hypercube Sampling (LHS) or Monte Carlo sampling are very computationally intensive, and can require significant amounts of time—needing on the order of thousands to tens of thousands of time-consuming simulations—to converge on a solution. Prof. Pitchumani and his NETL-RUA team in the Advanced Materials and Technologies Laboratory (www.me.vt.edu/amtl) at VT have developed a novel methodology—QUICKER: Quantifying Uncertainty In Computational Knowledge Engineering Rapidly—for speedily quantifying uncertainty in multiphase systems with minimal sampling. The QUICKER methodology requires significantly fewer simulations (on the order of tens of simulations) and orders of magnitude less computation time than conventional methods, without loss of accuracy. Figure 1 shows an example of a probability density function obtained from QUICKER (red line) in comparison to that from an LHS simulation (histogram) for uncertainty quantification on a three dimensional Circulating Fluidized Bed (CFB) scenario simulated by NETL's multiphase open source software MFIX. The QUICKER approach resulted in over 96% computational savings, with high accuracy quantified as a root mean square (RMS) error with respect to the histogram of about 3%.

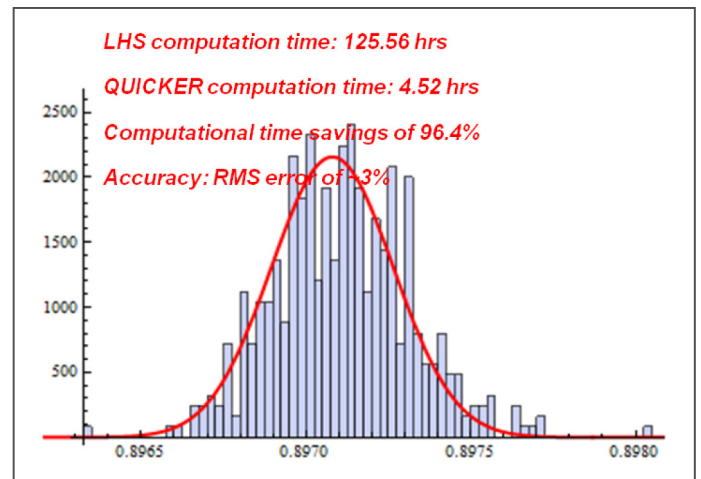


Figure 1. Comparison of LHS results (histogram) with QUICKER results (red line) for the 3D CFB scenario in MFIX.

Business Development Update

- ★ NETL has recently instituted Procedure 481.1, Reimbursable Work. (Reimbursable Work is services performed for or goods provided to an organization outside of NETL and the Office of Fossil Energy.) Reimbursable work performed by NETL is paid for by the customer, and states how NETL offices will engage in work for others. This reimbursable work procedure includes the execution of technology transfer agreements such as CRADAs, Contributed Funds Agreements (CFAs), any solicitation response where NETL is the proposal lead or partner, and any other outreach or business development activity, opportunity, or agreement that provides funding to NETL. All NETL-RUA members participating in a business development activity with NETL need to contact NETL's business development team for instructions on how to proceed in order to ensure compliance with Procedure 481.1. Key Business Development team contacts are as follows:

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- ★ NETL, URS, and other NETL-RUA members are working together to develop a response to a proposal for an Energy Innovation Hub for Critical Materials under Federal Opportunity Announcement number DE-FOA-0000687. This opportunity is worth approximately \$120 million over a five-year period and addresses issues associated with ensuring a stable supply of materials (rare earth elements and others) critical to energy applications. VT is leading the effort on behalf of NETL-RUA, and URS is supporting the effort with proposal management and technical writing resources. The Letter of Intent was submitted June 29, 2012 by VT, and the team has subsequently been asked to submit a full proposal.