netlognews

NETL's R&D newsletter *October 2011, Issue 23*

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U.S. DEPARTMENT OF ENERGY | the ENERGY lab
NATIONAL ENERGY TECHNOLOGY LABORATORY

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Cover image: Dr. Jinichiro Nakano, a URS scientist at work in the lab at NETL, will receive a 2011 Gustav Eirich Award.

newlognews is a quarterly newsletter that highlights recent achievements and ongoing research at NETL. Any comments or suggestions, please contact Paula Turner at paula.turner@netl.doe.gov or call 541-967-5966.

NETL to Investigate Hydrate Phenomena

—The U.S. Bureau of Ocean Energy Management, Regulation and Enforcement (BOEMRE) recently chose an NETL-led team to conduct laboratory experiments and thermodynamic, kinetic, and plume modeling to study the role that gas hydrate formation plays in the release and transport of hydrocarbons associated with deep-water well leaks.

The BP Macondo Well blowout in the Gulf of Mexico exposed significant gaps in our knowledge on how gas hydrate formation at such depths can affect the hydrodynamic and thermodynamic behavior of hydrocarbon fluids. NETL's high-pressure water tunnel facility (HWTF) allows researchers to simulate temperature and pressure at underwater depths to 3,400 meters, over twice that of the depth at which the Macondo release occurred.

The research team includes scientists and engineers from NETL, URS, NETL's Regional University Alliance, the Colorado School of Mines Center for Hydrate Research, and the University of California Santa Barbara. Experiments will be performed in the HWTF with hydrocarbon gas mixtures spanning compositions commonly encountered in deep reservoirs, including those in the Macondo reservoir. The researchers will also use oil drops saturated with similar hydrate-forming gases. These fluids will be injected into a countercurrent flow of artificial seawater in the HWTF to determine their fate and how hydrate formation affects their behavior and transport through the deep-sea water column.

The effects of dispersants and/or anti-agglomerants also will be studied. Using the experimental data, the team will refine thermodynamic, kinetic, and plume models relevant to deep-water releases of hydrocarbon fluids. The plume model will be applied to a range of simulated oil blowout plumes to describe the fate of released hydrocarbons and to provide testable hypotheses that can be confirmed with measurements at natural hydrocarbon seeps.

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New Technologies Bolster Function of Prosthetic Limbs

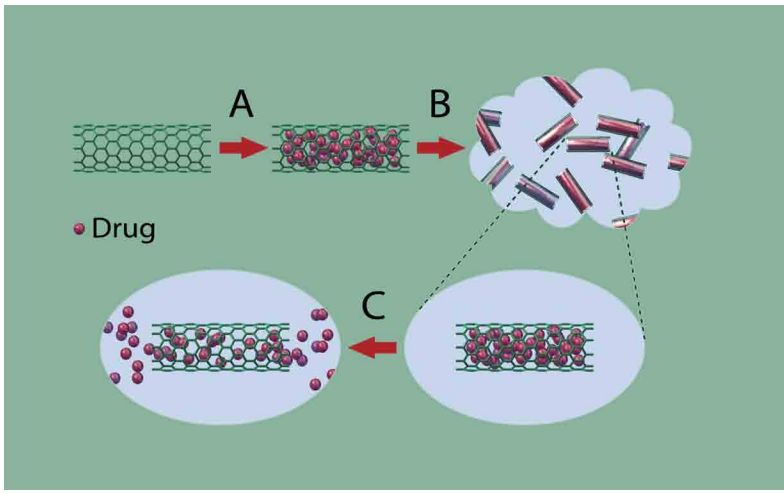
—A team of scientists from NETL and the University of Pittsburgh's Bioengineering Department are using new forms of nanotechnology to improve neural-controlled prosthetic implants. These technologies are of particular interest to the U.S. military for treating soldiers and veterans who have suffered loss of a limb during service. Neural-controlled prosthetics allow recipients to manipulate their artificial limbs by means of microelectrode implants placed in the brain or in other neural tissue.

One major barrier limiting the development of these prosthetics is decreased performance over time due to rejection of the microelectrode implant, the formation of scar tissue at the neural implant, or the loss of neural tissue in areas surrounding the implant. Microelectrode implants that can delivery anti-inflammatory drugs and other anti-rejection medicines in the vicinity of the electrode are being explored to improve these prosthetic devices.

The NETL and PITT-Bioengineering team addressed the controlled release of anti-inflammatory drugs for implant applications using drug delivery devices based on carbon nanotubes. The carbon nanotubes are about 10 nanometers wide and 50 micrometers long making them attractive for storing and delivering small quantities of drugs directly to the implantation site. These carbon nanotubes are also electrically conductive and can be chemically functionalized to facilitate the interaction of the drug with the carbon nanotube.

The collaborative research team investigated a series of carbon nanotubes and was able to demonstrate that carbon nanotube-based drug delivery systems outperformed standard delivery systems by improving the amount of drug released during electrical stimulation and increasing the lifetime of the drug delivery device. The released drug was then tested for bioactivity in live cell cultures, which had improved lifetimes as a result of the drug delivered from the carbon nanotube devices. The results of this study were recently published in the very high-impact factor journal, *Biomaterials* (Vol. 32, pp. 6316-6323).

Contact: Christopher Matranga, 412-386-4114



Schematic of the drug loading and release process of the carbon nanotube (CNT) nanoreservoirs.

A. Drug solution is filled into the interior of acid treated CNTs through sonication.

B. Pyrrole is added to the suspension containing CNTs and Dex and electropolymerization is carried out.

C. Drug is released from CNT nanoreservoirs to surroundings through diffusion or electric stimulation.

NETL Scientist Wins 2011 Gustav Eirich Award

—Congratulations to Dr. Jinichiro Nakano, a URS scientist at NETL, who will receive a 2011 Gustav Eirich Award. The Gustav Eirich Award was established to recognize outstanding young researchers in the field of refractory materials development. It is designed to promote the excellence of young academics and support innovative ideas in the refractory industry. Awards are given based on the applicant's presentation of environmental aspects, energy and other resources; the potential for significant impacts in the industry, design, and modeling for practical application; and the processing aspects of the development. The goal of the award is to advance contributions to the long-term success of companies in the refractory production and application industries.

Dr. Nakano was recognized for his NETL research on thermodynamic modeling of coal-petcoke slag compositions and its impact on refractory performance in slagging gasifiers. He will receive this award at the 54th International Colloquium on Refractories in Aachen, Germany, where he will present this research. The research also will be published in an upcoming issue of *refractories WORLDFORUM* — a new technical and scientific journal for the entire refractories sector: production, application, and further development of high-temperature materials.

Dr. Nakano is the first U.S.-based researcher to win this award.

Contact: David Alman, 541-967-5885

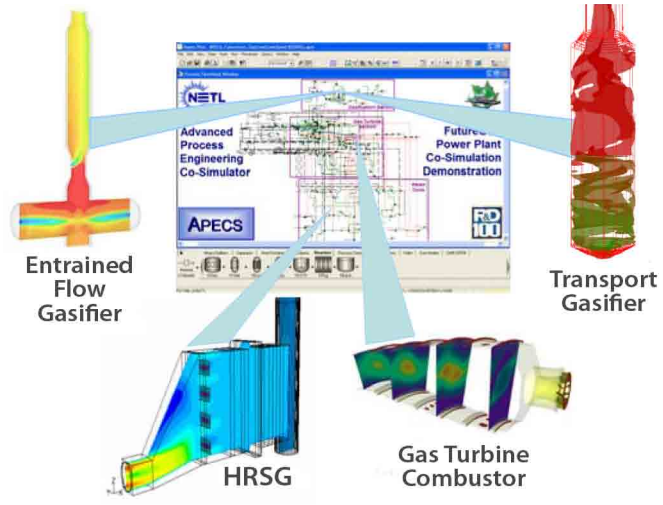
Researcher Recognized for Work in CO_2 Utilization

—Maria Salazar-Villalpando's paper, "CO_2 Electrochemical Reduction via Adsorbed Halide Anions," has been selected by the TMS Energy committee as the Best Paper from energy papers published in the 2011 TMS proceedings for the *JOM* magazine (a publication of the Minerals, Metals, and Materials Society). In this article, the electrochemical reduction of CO_2 to ethylene was described at ambient temperature and pressure. CO_2 emissions to the environment may be decreased via CO_2electrochemical conversion to high value products. This process may represent a technology for CO_2 utilization because it is simple and enables the production rate to be quickly varied to follow time-of-day availability of surplus electricity.

The reduction of CO_2 was conducted using copper and halide anions to facilitate the electron transfer from the electrode to CO_2. Results indicated that the stronger the adsorption of these halide anions to the electrode, the more strongly CO_2 was restrained, resulting in a higher CO_2 reduction current and a higher CO_2 conversion rate.

Moreover, adsorption of halide anions onto the working electrode may avoid hydrogen evolution—a competing reaction—by suppressing the adsorption of protons, promoting greater CO_2 electrochemical reduction.

Contact: Maria D. Salazar-Villalpando, 304-285-5427



APECS co-simulation of an advanced gasification-based power plant with carbon capture.

NETL's APECS Co-simulation Technology Highlighted in CAPE-OPEN Presentation

—NETL's 2011 R&D 100 award-winning Advanced Process Engineering Co-Simulator (APECS) was featured in a conference presentation given by Dr. Michel Pons, the Technology Officer of the CAPE-OPEN Laboratories Network (CO-LaN). Representing over 90 member organizations including NETL, CO-LaN is an internationally recognized user-driven organization for testing and management of the CAPE-OPEN standard. The standard defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications or components to interoperate. The presentation described how APECS v2.0 is built on this international standard, which provides plug-and-play model interoperability. Using APECS v2.0, design engineers can integrate, solve, and analyze co-simulations combining CO-compliant equipment simulations (e.g., gasifiers, CO_2 capture devices) with CO-compliant process simulations, such as for an IGCC power plant.

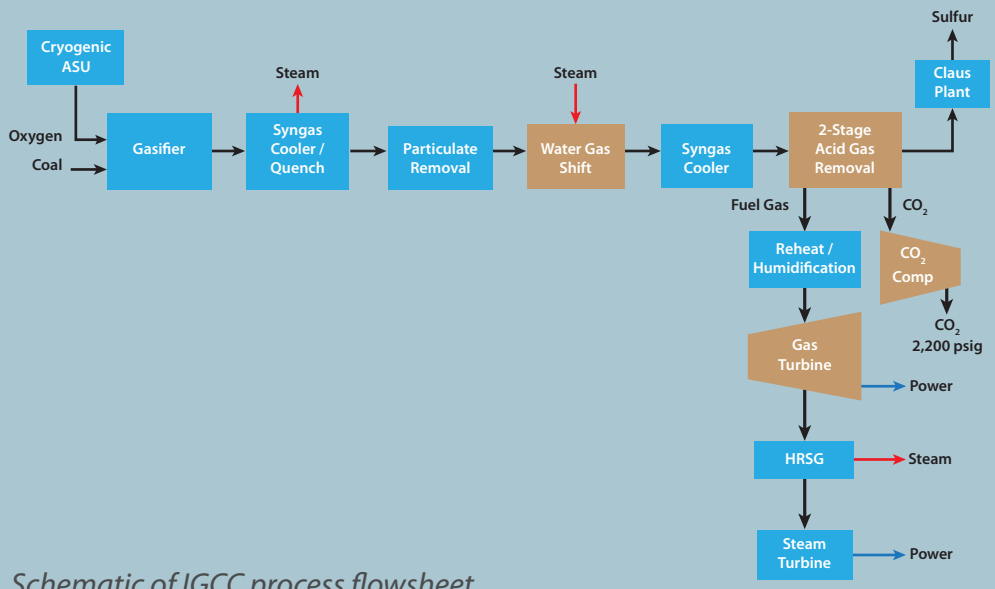
APECS provides easy-to-use configuration wizards for efficient configuration of CO-compliant equipment models, including high-fidelity computational fluid dynamics (CFD) models and fast reduced order models based on previous CFD results. The open, multi-platform CO interfaces are available free of charge and supported by many of the leading commercial process simulators.

Contact: Stephen E. Zitney, 304-285-1379

National Risk Assessment Partnership holds Initial Stakeholder Group Meeting

—The National Risk Assessment Partnership (NRAP), part of DOE's Carbon Capture and Sequestration Simulation Initiative (C2S2I), represents the best modeling and validation capabilities of five national labs (NETL, LANL, LBNL, LLNL, and PNNL). The NRAP Stakeholders Group is composed of industrial and academic experts in the field of carbon sequestration and risk management, and was formed to provide project direction and focus to the NRAP team. The initial NRAP Stakeholders Group meeting was held July 26-27, 2011, in Washington, DC. Members of the NRAP Leadership Team gave presentations on the goals of the project and the status of the working group activities. Valuable discussions were held on the details and the quality of the work being performed. The initial feedback from the Stakeholders group included praise for the quantity and quality of the work being performed.

Contact: Grant Bromhal, 304-285-4688



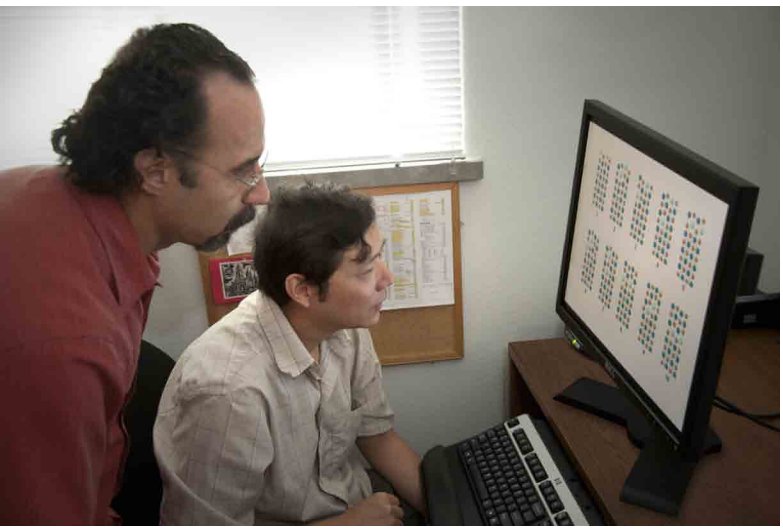
Schematic of IGCC process flowsheet.

Research Team Develops/ Demonstrates Models to Optimize IGCC

—For optimal overall power plant design and operation, computational fluid dynamics (CFD) models are required to capture spatially distributed phenomena in equipment items such as gasifiers, combustor, and CO_2 capture devices, which include multi-phase fluid flow, multi-phase reaction kinetics, and interfacial heat, and mass transfer. However, CFD models can become prohibitively expensive when integrated within a process simulation, especially when embedded in recycle and optimization loops. As a result, a systematic and effective approach is needed to generate reduced order models (ROMs) that significantly reduce the computational time and yield approximately the same fidelity as the CFD model.

To address these issues, NETL sponsored a collaborative Regional University Alliance project with researchers from Carnegie Mellon University to develop a ROM-based framework for the optimization of large-scale energy systems. As described in a recent issue of the Elsevier journal, *Computers & Chemical Engineering*, the ROMs derived from both gasification and gas turbine combustion units can be integrated within an equation-oriented simulation environment for the overall optimization of an IGCC process. The results of the ROM-based process optimization for an IGCC system with carbon capture show that the power output of the process can be increased by 5-7 percent compared to conventional process models.

Contact: Stephen E. Zitney, 304-285-1379



Computational Methods Used to Study Dissolution of Engineered Biomaterials

—Researchers at NETL and the University of Pittsburgh are applying skills and experience gained from studying energy-related materials to biomaterials. Magnesium (Mg) has attracted the attention of the biomaterials community as a potential biodegradable metallic candidate for use in stents and orthopedic applications. Magnesium has properties such as density, elastic modulus, strength, and toughness, which are more similar to the properties of natural bone than other implant metallic materials (stainless steel, titanium, and cobalt-chromium based alloys). Most importantly and intriguingly, Mg dissolves in human blood plasma. Controlled corrosion of an Mg implant could eliminate the need to surgically remove the implant, reducing costs for the health care system and morbidity for the patient. Alloying Mg with other metals is important to optimize its corrosion rate.

The research team investigated the chemical reactions of Mg alloys with pure water using calculations based on phase diagrams (CALPHAD). A qualitative agreement between CALPHAD and first-principles results was obtained. The CALPHAD method was also used to study the reactions of Mg alloys in the human blood fluid environment. The effects of alloying elements and compositions on the reaction enthalpies, reaction products, amount of gas release, and gas compositions as well as the pH of the fluids was recently systematically discussed and reported in *Materials Science and Engineering B.*

Contact: Omer Dogan, 541-967-5858 and Kaisheng (Kevin) Wu, 541-967-4421

Wyoming Geophysical Survey Completed for Potential Use of Produced Water

—An investigation is ongoing for potential uses for water produced during extraction of coal bed natural gas (CBNG). Another ground-based multi-frequency electromagnetic survey was conducted at the Headgate Draw Subsurface Drip Irrigation (SDI) installation, which is located at the confluence of Crazy Woman Creek and the Powder River in Wyoming. These SDI systems beneficially use the CBNG produced water, safely irrigating agricultural lands.

The electromagnetic response measured by NETL researchers serves as a proxy to monitor near-surface soil salinity. Repeat surveys are necessary to detect changes in salinity resulting from seasonal variations in hydrologic condition, water application rate, precipitation events, and crop transpiration.

These data are shared with our U.S. Geological Survey collaborators and will be used to refine current inversion models of the subsurface that should improve irrigation management and minimize potential impacts.

Contact: Garret Veloski, 412-386-5809 and Jim Sams, 412-386-5767

Recent NETL Publications

1.	Tsai, A., Tucker, D., and Groves, C. July 2011. Improved Controller Performance of Selected Hybrid SOFC-GT Plant Signals Based on Practical Control Schemes, *Journal of Engineering for Gas Turbine and Power-Transactions* of the ASME, 133(7) No. 071702.
2.	Zhong, Z., Amrinder, G., Dong, Q. et al. A Finite Element Study of Thermal Relaxation of Residual Stress in Laser Shock Peened IN718 Superalloy, Intl. *Journal of Impact Engineering*, 38(7) 590-596.
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5.	Mehrdad, M.A. July 2011. A Generalization of Reiner's Mathematical Model for Wet Sand, *Mechanics Research Communications*, 38 (5) 378-381.
6.	Junseok, L., Sorescu, D.C., and Xingyi, D. July 201. Electron-Induced Dissociation of CO(2) on TiO(2)(110) *Journal of the American Chemical Society*, 133 (26) 10066-10069.
7.	Lopano C. L., Heaney, P.J., Bandstra, J.Z.; et al. July 2011. Kinetic Analysis of Cation Exchange in Birnessite Using Time-Resolved Synchrotron X-ray Diffraction, *Geochimica et Cosmochimica Acta*, 75(14) 3973-3981.
8.	Ferer M., Crandall, D., Goodarz, A. et al., July 2011. Two-Phase Flow in a Rough Fracture: Experiment and Modeling, *Physical Review E*, 84 (1) No. 016316.
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10.	Cowen, C.J., Danielson, P.E., and Jablonski, P.D. August 2011. The Microstructural Evolution of Inconel Alloy 740 During Solution Treatment, Aging, and Exposure at 760 A degrees C, *Journal of Materials Engineering and Performance,* 20(6), 1078-1083.
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12.	Ciferno J. P., Marano, J. J., Munson, R.K. August 2011. Technology Integration Challenges, *Chemical Engineering Progress,* 107(8) 34-44.
13.	Zheng P., Chin, T.-L., Greve, D., et al. August 2011. High-Temperature Langasite SAW Oxygen Sensor, *IEEE Transactions on Ultrasonics Ferroelectrics and Frequency* Control, 58 (8) 1538-1540.
14.	Seol, Y., Kneafsey, T.J. August 2011. Methane Hydrate Induced Permeability Modification for Multiphase Flow in Unsaturated Porous Media, *Journal of Geophysical Research-Solid Earth*, 116, No. B08102.
15.	Mahalatkar, K., Kuhlman, J., and Huckaby, E. D. et al. August 2011. CFD Simulation of a Chemical-Looping Fuel Reactor Utilizing Solid Fuel, *Chemical Engineering Science*, 66 (16) 3617-3627.

Recent NETL Publications

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17.	Karaivanov, V. G., Slaughter, W.S., Siw, S., et al. September 2011. Compressive Creep Testing of Thermal Barrier Coated Nickel-Based Superalloys, *Journal of Engineering for Gas Turbines and Power-Transactions of The ASME*, 133 (9), No. 091301.
18.	Jones, D., Bhattacharyya, D., Turton, R., et al. September 2011. Optimal Design and Integration of an Air Separation Unit (ASU) for an Integrated Gasification Combined Cycle (IGCC) Power Plant with CO(2) *Capture, Fuel Processing Technology*, 92 (9) 1685-1695.
19.	Luo, X., Matranga, C., Tan, S., et al. September 2011. Carbon Nanotube Nanoreservior for Controlled Release of Anti-Inflammatory Dexamethasone, *Biomaterials* 32(26) 6316-6323.
20.	Alfonso, D.R. September 2011. Computational Studies of Experimentally Observed Structures of Sulfur on Metal Surfaces, *Journal of Physical Chemistry C*, 115 (34) 17077-17091.
21.	Voora, V.K., Al-Saidi, W.A., Jordan, K. D. September 2011. Density Functional Theory Study of Pyrophyllite and M-Montmorillonites (M = Li, Na, K, Mg, and Ca): Role of Dispersion Interactions, *Journal of Physical Chemistry A*, 115(34) Special Issue, 9695-9703.
22.	Harendra, S., Oryshchyn, D., Ochs, T. et al. September 2011. Coagulation/Flocculation Treatments for Flue-Gas-Derived Water from Oxyfuel Power Production with CO(2) Capture, *Industrial & Engineering Chemistry Research*, 50(17) 10335-10343.
23.	Salazar, J.M., Diwekar, U.M., Zitney, S.E., September 2011. Rigorous-Simulation Pinch-Technology Refined Approach for Process Synthesis of the Water-Gas Shift Reaction System in an IGCC Process With Carbon Capture, *Computers & Chemical Engineering*, 35(9), Special Issue, 1863-1875.
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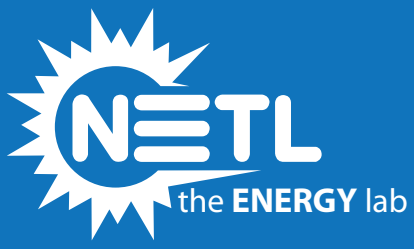

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