

#### APRIL 2021

# U.S. DEPARTMENT OF ENERGY | OFFICE OF FOSSIL ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY



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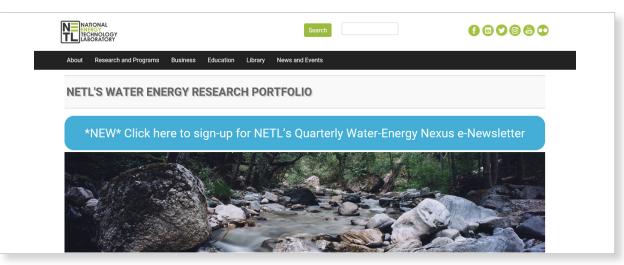
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### NETL's Water-Energy Nexus e-Newsletter Sign-Up Button



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### NETL Welcomes DOE's Office of Fossil Energy's New Water Management R&D Team

#### Sotirios (Sam) Thomas

Director, Advanced Energy & Hydrogen Systems, Acting Program Manager for Sensors & Controls and Novel Concepts, Acting Program Manager for Water Management R&D

As the Director of the Advanced Energy and Hydrogen System (AEHS) Program at the Office of Fossil Energy, Sam Thomas oversees the planning, management and execution of research and development. AEHS plays an integral role in DOE's leadership toward meeting the challenge of decarbonizing fossil-based power plants, deploying zero-carbon hydrogen production and utilization technologies, and achieving a carbonfree power sector by 2035. Thomas is charged with managing and facilitating interdisciplinary cutting-edge research and development in efficient and cost-effective technology to meet energy and environmental requirements domestically and internationally. The AEHS division includes seven R&D portfolios with the goal of improving overall system efficiency, reducing capital and operating costs, and enabling affordable carbon capture. The portfolios include (1) Hydrogen; (2) Advanced Gasification (3) Advanced Turbines; (4) Solid Oxide Fuel Cells (SOFCs); (5) Advanced Sensors and Controls; (6) Water Management R&D; and (7) Advanced Energy Materials.

#### Hichem Hadjeres Project Coordinator, Water Management R&D

Hichem Hadjeres supports the Director and coordinates day-to-day operations of the AEHS Water Management program. Hadjeres also collaborates closely with NETL and other DOE organizations in the planning and execution of water R&D projects, focusing on performance optimization, water use reduction, and emissions control.

# Highlights: NETL Hosts a Webinar to Present the New ProteusLib at NAWI

In February 2021, NETL Senior Fellow for Strategic Systems Analysis and Engineering (SSAE), David Miller, provided an overview of ProteusLib, a new, open-source library of water-specific models being created as part of the AMO-funded National Alliance for Water Innovation (NAWI). Miller was assisted by fellow SSAE researchers Timothy Bartholomew and Markus Drouven, along with collaborator Deb Agarwal at Lawrence Berkeley National Laboratory. ProteusLib is built on NETL's Institute for the Design of Advanced Energy Systems (IDAES) Integrated Platform, which enables advanced modeling and optimization for (1) conceptual design, (2) multiscale design, and (3) dynamics and model predictive control of systems and networks. The new capabilities of ProteusLib will support the design and optimization of integrated water treatment systems to improve existing systems and



enable the analysis of innovative new designs that incorporate emerging technologies. ProteusLib is scheduled to be released later this year.

For more information on IDAES, visit https://idaes.org.

To watch the recorded presentation, visit https://www. nawihub.org/archives or click here.

### Highlights: NETL Engages with the Southwestern Pennsylvanian Commission's Water Resource Center

As part of the ongoing efforts to engage with national and regional water-energy stakeholders, NETL recently spoke with Erin Kepple Adams, manager of the Southwestern Pennsylvania Commission's Water Resource Center about the laboratory's water-energy nexus research and development (R&D) activities.

The Southwestern Pennsylvania Commission is comprised of a 60-plus-member governing body and a 50-plusmember administrative arm – all working together on the goals of transportation, planning and development, and information systems in the Southwestern Pennsylvania region. This includes the following: the city of Pittsburgh, Allegheny County, Armstrong County, Beaver County, Butler County, Fayette County, Greene County, Indiana County, Lawrence County, Washington County, and Westmoreland County.

The Water Resource Center (WRC) promotes regional collaboration on water topics, and has four major tasks: (1) to provide technical assistance, (2) to provide educational resources, (3) to serve as a regional information clearinghouse, and (4) to provide a forum for regional coordination of water issues. A key tool offered by the WRC is its interactive Water-Related Plans and Reports



Southwestern Pennsylvania Commission

Tool for locating important information on a particular watershed or county-wide plans in the Southwestern Pennsylvania region. The tool allows users to gather data from existing regional water resource plants, to identify funding priorities, and to support the development of grant or loan applications.

The WRC is interested in learning more about NETL's research in recovering rare earth elements (REE) and critical materials (CM) from acid mine drainage (AMD). AMD remains a serious environmental concern in Southwestern Pennsylvania and surrounding regions, with many communities not having adequate resources to address the problem. The potential to recover REE/CM as a revenue stream to offset the cost of AMD treatment may offer a future collaborative opportunity between WRC and NETL.

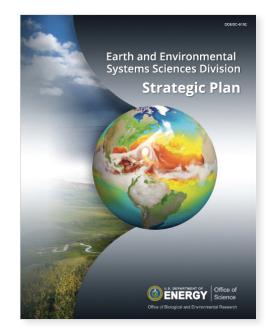
For more information on Water Resource Center, visit https://spcwater.org.

### Highlights: NETL Participates in DOE's Call for White Papers to Advance an Integrative Artificial Intelligence Framework for Earth System Predictability

The DOE's Earth and Environmental Systems Sciences Division (EESSD), within the Office of Science's Biological and Environmental Research (BER) program, has issued a call for white papers. The white papers are intended to "inform the design of three sequential workshops (conducted in 2021–2022) focused on answering the following overarching question of: How can DOE directly leverage artificial intelligence (AI) to engineer a substantial (paradigm-changing) improvement in earth system predictability?"

Nearly a decade ago, the DOE recognized that an acceleration was needed in the transition of basic science into new predictive capabilities. To help meet this challenge, EESSD incorporated a novel model-experiment (MODEX) approach, linking interdependent observation and model development into its management philosophy and strategic planning.

The DOE's vision is to make radical improvements in predictive capabilities by applying AI methods to build a new integrative system that spans the continuum from observations to predictive modeling, particularly related to the integrative water cycle and associated water cycle extremes. This effort will require the exploration of AI across the MODEX enterprise to determine the most impactful applications along the observation-modeling continuum.



NETL coordinated two white papers for this call. Kelly Rose, Ph.D., Interim Technical Director of Science-Based Artificial Intelligence and Machine Learning Institute, is the lead for the "Data Acquisition and Assimilation" paper. Grant Bromhal, Ph.D., Senior Fellow of Geological and Environmental Systems, is the lead for the "Insight Gleaned from Complex Data Focus on Science-informed Machine-learning to Accelerate Real Time (SMART)" paper.

For more information on the white papers, visit https:// climatemodeling.science.energy.gov or click here.

For more information on SMART, visit https://edx.netl. doe.gov/smart.

### Highlights: DOE-FE Selects Additional Projects Seeking Beneficial Uses for Coal Combustion Residuals

In March 2021, the DOE announced the selection of two projects to receive approximately \$2 million in federal funding for cost-shared R&D. The projects will improve Coal Combustion Residuals (CCR) management under the funding opportunity announcement (FOA) DE-FOA-0002190, Research for Innovative Emission Reduction Technologies Related to Coal Combustion Residuals.

These selected projects represent the second round of selections for the FOA. The first round of selections were made in July 2020.

CCR consists primarily of fly ash, bottom ash, boiler slag, flue gas desulfurization (FGD) gypsum, and other FGDsolid by-products, as well as fluidized bed combustor ash from pulverized coal-fired power plants and other combustion-based coal power plants.

R&D under this FOA aims to advance the management of CCR impoundments with the goal of increasing the beneficial reuse of these materials while protecting the environment by preventing the potential release of metals and other contaminants found in CCR into ground and surface water. These projects are highlighted below:

Beneficial Use of Harvested Ponded Fly Ash and Landfilled FGD (Flue Gas Desulfurization) Materials for High-Volume Surface Mine Reclamation — The Ohio State University (Columbus, Ohio)

The project intends to focus on the viability of beneficial use of harvested CCRs, especially ponded fly ash and landfilled FGD by-products in the vicinity of coal ash pond facilities and FGD landfills, and demonstrate the laboratory- and bench-scale testing and construction methods.

#### Surface Modified Fly Ash for Value Added Products (SuMo Fly Ash) — University of Illinois (Champaign, Illinois)

The University of Illinois plans to develop a technology to encapsulate coal fly ash particles in sulfurized vegetable oil, enhancing physical and mechanical properties of the fly ash as a filler material when applied in commercial products that will increase cross-linking, compatibility and air-entrainment, and decrease the leaching potential of metals of concern.

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# Water-Energy Project Highlights

Through the DOE's Carbon Capture, Utilization, and Storage R&D Program, the Office of Fossil Energy has selected 27 projects for cost-shared R&D under two separate FOAs. While focusing on advanced technologies for the removal of carbon dioxide ( $CO_2$ ) from manufacturing and industrial sources (FOA DE-FOA-0002187) and the direct capture of  $CO_2$  from the atmosphere (FOA DE-FOA-0002188), the projects also offer the potential to separate, recover, and reuse water. These projects are described below:

#### Next Generation Fiber-Encapsulated Nanoscale Hybrid Materials for Direct Air Capture with Selective Water Rejection

Columbia University and its project partners will develop a tailored sorbent material in combination with state-of-the-art anhydrous nanofluid solvent and electrospinning technology

to form a hybrid coaxial-fiber system for direct air capture (DAC) of  $CO_2$ . The nanofiber-encapsulated sorbent has the ability to selectively reject water while allowing facile  $CO_2$  diffusion, which can lead to a reduction in parasitic energy consumption during pressure/temperature swing desorption. The project team will investigate underlying mechanisms that impact sorption kinetics, thermodynamics, and mass transfer to gain an understanding that will enable tuning key parameters of encapsulated hybrid coaxial fiber for optimal operating conditions in DAC.

Columbia | Engineering

The Fu Foundation School of Engineering and Applied Science

#### A Combined Water and CO<sub>2</sub> Direct Air Capture System

IWVC, LLC, along with its team plan to design, manufacture, and field test a combined water and CO<sub>2</sub> DAC system at a field site located on the San Diego State University Brawley campus. The team's ultimate goal is to demonstrate the technical and economic performance of a transformational technology that simultaneously captures CO<sub>2</sub> and water from the air.

For more information on the FOAs, visit https://www.energy.gov/fe or click here. To learn more about NETL's fossil energy R&D awards, visit https://netl.doe.gov or click here.

# **Conferences and Events**

Listed below are of upcoming conferences and events that align with the Laboratory's water-energy research efforts.

#### The Water Expo

**Description:** The Water Expo is a bilingual tradeshow and conference that presents equipment, technologies, products & know-how for the wastewater, sewer infrastructure, environmental services, portable sanitation, water quality, and high-pressure industries. There will be a virtual conference in May 2021 and an in-person conference in August 2021 in Miami, FL.

Date: May 3–7, 2021 and Aug. 25–26, 2021 Locale: Virtual + In-Person (Miami, FL) Website: https://www.thewaterexpo.com

#### 2021 World Environment & Water Resources Congress

**Description:** Attendees at the EWRI Congress in Milwaukee will have the opportunity to share their research on issues affecting the environment and the policies relating to water resources. As a water community, we will focus on using our existing knowledge, combined with fresh ideas to maximize resources and develop best practices as we strive for a healthy future environment.

Date: June 7–11, 2021 Locale: Virtual Website: https://www.ewricongress.org

# AWRA's 2021 Virtual Summer Conference: Connecting Land & Water for Healthy Communities

**Description:** The American Water Resources Association (AWRA) conference aims to bring together stakeholders across multiple disciplines and types of organizations and professions to address the design, integration, and implementation of the programs necessary to better connect land and water planning and policy. Topics will include land and water aspects of water supply, water demand management, stormwater management, wastewater treatment, community planning and design, conservation, and integrated "one water" approaches.

Date: July 19–21, 2021 Locale: Virtual Website: https://www.awra.org/Members/Events\_and\_Education/Events/2021\_Summer\_Conference

#### **Clearwater Clean Energy Conference**

**Description:** Increased demand coupled with energy security issues, uncertainty in the oil sector, and tightening environmental regulations make this conference a must for those involved in all aspects of power generation. The conference will present an extensive overview of emerging, evolving, and innovative technologies, fuels and/or equipment in the power generation industry. NETL's Thermal Sciences Team Supervisor, Ronald Breault serves as one of the committee cochairs.

Date: July 25–29, 2021 Locale: Virtual + In-Person (Clearwater, FL) Website: http://clearwatercleanenergyconference.com

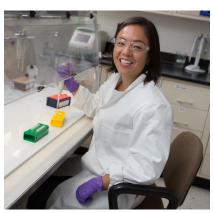
## **Researcher Spotlight**



#### **Djuna Gulliver** Environmental Engineering Researcher djuna.gulliver@netl.doe.gov

Djuna Gulliver, Ph.D. is an Environmental Engineering Researcher on the Geochemistry Team. She completed her Ph.D. in Environmental Engineering from Carnegie Mellon University, master's in Environmental Engineering from Johns Hopkins University, and bachelor's in Chemical Engineering, Geology, and Geophysics from University of Minnesota.

Gulliver's research focuses on microbiology of water related to energy and energy waste streams. Her work involves characterizing how microbiology that naturally inhabit reservoir fluids affect reservoir properties through microbial processes such as biocorrosion, biomineralization, metal mobilization, and metal immobilization. Along with her team, Gulliver has demonstrated how the microbial ecology of the subsurface waters can change conditions in  $CO_2$  storage reservoirs, coalbed methane deposits, and unconventional oil and gas reservoirs. They are also conducting research to use these microorganisms to catalyze reactions that can help treat energy waste streams.



#### <sup>66</sup>Our microorganisms are currently capable of treating flue gas desulfurization effluent and upgrading CO<sub>2</sub> to value-added products. Many of these microorganisms are the same that we collect from the subsurface; we just harvest and enrich for them to perform treatment processes.<sup>99</sup>

Gulliver was also directly involved in the NAWI road mapping group for resource extraction. In addition to her NAWI effort, Gulliver recently submitted a proposal with the U.S. Geological Survey researchers on investigating microbiology of energy systems.

Gulliver has co-authored 14 scientific publications including a conference paper. Her most recent publications include Predominance and Metabolic Potential of Halanaerobium in Produced Water from Hydraulically Fractured Marcellus Shale Wells and Comparative Study of Effects of CO<sub>2</sub> Concentration and pH on Microbial Communities from a Saline Aquifer, a Depleted Oil Reservoir, and a Freshwater Aquifer. Her water-related effort includes the waterwaste treatment technology under FWP task Biological Treatment of FGD Effluent Streams (FWP-1022428 Task 6).

## **Recent Water-Related Publications** and Presentations

Below are several water-related journal articles authored or co-authored by NETL staff.

#### Observations of Breakage for Transversely Isotropic Shale Using Acoustic Emission and X-Ray Computed Tomography: Effect of Bedding Orientation, Pre-Existing Weaknesses, and Pore Water

Guanyi Lu, ORISE/NETL; Dustin Crandall, NETL; Andrew P. Bunger, University of Pittsburgh (MARCH 2021) https://www.sciencedirect.com/science/article/abs/pii/S136516092100037X

# Characterizing Mineralization on Low Carbon Steel Exposed to Aerated and Degassed Synthetic Hydraulic Fracture Fluids

Justin Mackey, Leidos/NETL; James B. Gardiner, Leidos/NETL; Barbara Kutchko, NETL; Meghan Brandi, ORISE/ NETL; James Fazio, Leidos/NETL; J. Alexandra Hakala, NETL (FEBRUARY 2021)

▶ https://www.sciencedirect.com/science/article/abs/pii/S092041052100173X

#### Predicting the Potential for Mineral Scale Precipitation in Unconventional Reservoirs Due to Fluid-Rock and Fluid Mixing Geochemical Reactions

J. Alexandra Hakala, NETL; Amelia N. Paukert Vankeuren, ORISE/NETL; Peter P. Scheuermann, ORISE/NETL; Christina Lopano, NETL; George D. Guthrie, Los Alamos National Laboratory (JANUARY 2021)

▶ https://www.sciencedirect.com/science/article/abs/pii/S0016236120318792

#### Tracking Natural CO<sub>2</sub> Migration Through a Sandstone Aquifer Using Sr, U and C Isotopes: Chimayó, New Mexico, USA

James B. Gardiner, NETL; Rosemary C. Capo, University of Pittsburgh; Dennis L. Newell, Utah State University; Brian W. Stewart, University of Pittsburgh; Thai T. Phan, University of Pittsburgh; Elizabeth H. Keating, Los Alamos National Laboratory; George D. Guthrie, Los Alamos National Laboratory; J. Alexandra Hakala, NETL (JANUARY 2021)

▶ https://www.sciencedirect.com/science/article/pii/S1750583620306344

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626 Cochrans Mill Road P.O. Box 10940 Pittsburgh, PA 15236-0940 412-386-4687

Program staff are also located in **Houston, Texas,** and **Anchorage, Alaska.** 

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## **Get Social with Us**

There are several ways to join the conversation and connect with NETL's Water-Energy Research Program:



# Partnering with NETL

NETL's partnership activities are central to DOE's core mission. NETL utilizes a complete suite of contractual vehicles, as well as its inherent authority as a GOGO laboratory, to pursue technology development and eventual transfer of technology to the marketplace. NETL's success in developing technology solutions that can be applied to the intersection of water and energy depends upon strong relationships with both public and private entities. From targeted competitive announcements to cooperative research and development agreements, NETL offers a variety of cost-shared funding and partnership arrangements to help move technology and intellectual property through the maturation cycle into the marketplace.

For more information on partnering with NETL in the water-energy space, contact:

Thomas J. Feeley, III Research Partnerships & Technology Transfer Thomas.Feeley@netl.doe.gov 412-386-6134

https://netl.doe.gov/water-energy-research



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