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U.S. DEPARTMENT OF ENERGY AND CARBON MANAGEMENT | NATIONAL ENERGY TECHNOLOGY LABORATORY

An Update on the National Energy Technology Laboratory's Water-Energy Research and Related Activities

IN THIS ISSUE Highlights Researcher Spotlight In the News Publications

Highlights: Meet the National Energy Water Treatment & Speciation (NEWTS) Database Dashboard

Accurate data is crucial for determining the best way to manage industry generated wastewater. Because of the data's importance, researchers and computational science experts at the U.S. Department of Energy (DOE) National Energy Technology Laboratory (NETL) have developed the NEWTS Database Dashboard, a searchable spatial-visualization tool for investigating energy-related wastewater streams across the United States.

NEWTS is a first-of-its-kind research product that does more than simply inform decisionmaking regarding wastewater management. It also expands public access to wastewater data, encourages environmental responsibility and promotes the long-term stewardship



The NEWTS dashboard features an interactive map to pinpoint locations across the United States where samples of energy-process water have been collected and provides the water-quality test results from those samples.

of natural resources. Members of the public can use NEWTS to obtain records of toxins and chemicals that may contaminate the water sources they rely on. In addition, researchers can use NEWTS to investigate chemical reactions and physical processes that occur in aqueous environments, and policymakers can use it to pursue water-quality regulations and monitoring requirements that are effective and appropriate.

Through NETL's Energy Data eXchange, the public-facing side of NEWTS provides downloadable datasets for more than 2 million wells and power plants in the United States. By curating publicly sourced data into a uniform format, NEWTS makes it easier to obtain waste-stream compositions, volumes and locations, including geochemical data associated with produced water from oil and gas wells and power plant flue-gas-desulfurization effluent, including rare earth elements and critical minerals. Users can view datasets for the entire nation or just a specific region, state, county, subbasin, watershed, well, or power plant. They can also filter the data by various attributes, such as the date a water sample was collected or the number of dissolved aqueous species measured. The availability of this data in a simple format enables water-quality experts and related researchers to spend less time gathering and manipulating data, and more time conducting analyses, building models and designing water treatments.

The data that NEWTS aggregates will help mitigate environmental risks while identifying potential sources of critical minerals (CMs) and rare earth elements (REEs), which are necessary for manufacturing many of the batteries, magnets, catalysts and other technologies that underpin the nation's security, prosperity and energy independence. Rebuilding the domestic supply chain of these scarce materials can create jobs and spur economic growth. The development team envisions the project will drive the development of a circular economy in communities whose economies have historically depended on operating fossil-fueled power plants or developing the coal, oil and natural gas needed to run them.

Please visit NETL's YouTube channel to watch a new introductory video on the NEWTS Database Dashboard.

Highlights: NAWI Funds New Projects That Will Use State-of-the-Art Tool Developed at NETL



The National Alliance for Water Innovation (NAWI) announced awards of \$9 million for 12 research projects and \$5 million for 11 pilot-scale projects to advanced desalination and water reuse technologies. Four research projects and three pilot-scale projects are planning to use a software tool developed at NETL and other national labs called the Water treatment Technoeconomic Assessment Platform (WaterTAP).

NETL is leading one of the recently awarded research projects and is a contributor to another. The NETL-led project is evaluating the potential of recovering minerals from brackish water and repurposing waste brine. If successful, the project hopes to identify viable treatment trains that reduce brackish water desalination by creating sellable products. The other NETL project, led by Stanford University, seeks to assess the value of flexible operation for commercial-scale desalination plants with the primary benefit of reducing annual electricity costs by shifting demand throughout the day.

Highlights: WaterTAP Releases Version 0.9

WaterTAP is an open-source Python-based software tool for assessing the performance and economic viability of water treatment trains. The tool development began in July 2020 and is updated quarterly. The development is led by researchers at NETL in collaboration with other national labs including Lawrence Berkeley National Laboratory (LBNL), National Renewable Energy Laboratory (NREL) and Oak Ridge National Laboratory. The tool includes modeling, simulation and optimization capabilities for membrane, evaporative, adsorption and electrochemical processes.

The most recent releases in March and June 2023 included models for osmotically assisted reverse osmosis, electrocoagulation, electrolyzer, activated sludge processes and anaerobic digestor, as well as refinements to existing models and capabilities. For more on WaterTAP, see GitHub or documentation.

Highlights: Great River Energy Clean Coal Power Initiative Project Repayment Passed \$6 Million Mark; Technology Helps to Reduce Thermoelectric Power Plant Water Use

Through a project funded by NETL's Clean Coal Power Initiative (CCPI), Great River Energy (GRE) demonstrated a cost-effective technology for reducing emissions from coal-based power plants. As of May 2023, the project has repaid over \$6 million to DOE.

The project, "Lignite Fuel Enhancement" (DE-FC26-04NT41763), centered on DryFining, which reduces power plant emissions by improving fuel quality. DryFining utilizes a plant's waste heat (and a proprietary fluidized-bed drying process) to dry out and purify low-grade types of coal so that they perform more like their higher-grade counterparts. Doing so helps the coal burn more cleanly and efficiently. It also makes it easier to isolate and contain many of the pollutants generated by burning coal and uses less cooling water to generate electricity.

The initial feasibility study "Use of Coal Drying to Reduce Water Consumed in Pulverized Coal Power Plants" (DE-FC26-03NT41729) was conducted in 2002 at the Lehigh University Energy Research Center using a laboratory-scale fluidized bed dryer and was one of the first water projects from NETL's inaugural water-energy program initiated in 2002. Soon after, GRE tested DryFining in a pilot-scale coal-drying facility. GRE then designed, fabricated and tested a full-scale, commercial drying system at GRE's Coal Creek Station in North Dakota. As a result, GRE's Coal Creek Station lowered its sulfur dioxide and mercury emissions by 40 percent, its nitrogen oxide emissions by 20 percent and its carbon dioxide emissions by 4 percent. Additionally, GRE found that removing moisture from coal decreased its volume of exhaust gas and improved the efficiency of the station's fans, motors and emissions-control equipment.

Implemented by NETL, CCPI was a cost-shared collaboration between the federal government and private industry. It aimed to stimulate investment in low-emission coal-based power generation technologies through commercial demonstrations. GRE's demonstration of DryFining showed the technology's promise for improving efficiency in the energy sector.

Water-Energy Project Highlights: ZwitterCo, Inc., Demonstrates Membrane Technology to Cost-Effectively Treat Produced Water from Oil and Gas Wells



The left jar shows the wastewater stream sent through ZwitterCo's superfiltration membranes. The middle jar is the concentrate following membrane treatment. The right jar is the permeate from the membranes, enabling clean water for reuse.

Water scarcity is a growing concern worldwide, yet water is necessary for every phase of energy production and electricity generation. In particular, the drilling and hydraulic fracturing of oil and gas wells involves large volumes of water, which often come from rapidly diminishing sources. Reusing the water, rather than disposing of it, is one way to accomplish more with the dwindling water supplies available. But reuse requires extensive—and expensive—water treatment.

With nearly \$1.25 million in DOE funding, ZwitterCo, Inc., has developed a membrane technology that helps to lower these technical and economic hurdles. The technology at the heart of the project incorporates zwitterionic polymers, molecules that contain a positively and negatively charged functional group at either end. Zwitterionic polymers are noteworthy for their absorbency, resistance to fouling and ability to withstand very salty environments. ZwitterCo and its

project partners (Tufts University, Advisian, Heartland Water Technologies, the Brackish Groundwater National Desalination Research Facility, and Daniel Shannon) took advantage of these properties by incorporating the polymers into a superfiltration membrane module for treating produced water from the Permian Basin.

Produced water is the groundwater that accompanies oil and gas extracted from underground reservoirs. Typically, it is very salty and mixed with oil residues—making it difficult to reuse in fracturing new wells, operating power plants, irrigating crops, extinguishing wildfires or meeting other needs. ZwitterCo's two-year-project "Fouling-Resistant, Chlorine-Tolerant Zwitterionic Membranes for Treatment of Produced Water in the Permian Basin" showed that zwitterionic membranes can be a practical, cost-effective option for treating produced water.

Before the project concluded, ZwitterCo and its partners demonstrated their membrane module's ability to pretreat produced water for subsequent desalination. The module recovered 99% of the produced water, which came from the Permian Basin. It also achieved complete membrane cleanability and maintained an uptime of greater than 95%. Crucially, the module could treat the produced water inexpensively. Its superfiltration step costs an estimated \$0.11 per barrel, falling below the \$0.20-per-barrel threshold set by the New Mexico Produced Water Research Consortium (NMPWRC). After ZwitterCo and its partners accounted for the entire membrane-distillation process—and for additional transport and disposal needs—the levelized cost for beneficial reuse was \$1.54–1.94 per barrel of desalinated water. This levelized cost adheres to NMPWRC's criteria. It is also lower than the \$2-per-barrel cost that industry representatives (whom ZwitterCo interviewed) said would make a fully integrated treatment process economically viable in the Permian Basin.

This project is significant because the Permian Basin, which spans much of western Texas and southeastern New Mexico, accounts for about 43% of the nation's oil production and about 17% of its natural gas production.¹ Additionally, the amount of water that hydraulic fracturing consumes in the area—on a per-well basis—has surged over the past decade.² Reusing the produced water associated with these activities could have an outsize impact on both the energy industry and the environment.

ZwitterCo presented the results of the project at the Produced Water Society Seminar in February 2023. Christopher Drover, ZwitterCo's Chief Technology Officer, said many people expressed interest in the product after seeing what could be possible in produced water treatment. The company is currently working toward several pilots for 2023.

> 1. https://www.eia.gov/todayinenergy/detail.php?id=54079 2. https://pubs.usgs.gov/fs/2021/3053/fs20213053.pdf

In the News

A New Approach to Power Plant Cooling Can Eliminate the Need for Freshwater Use

Researchers at NETL and the University of Wyoming report that using brackish water—water containing 1,000–35,000 parts per million of dissolved solids and, therefore, unsuitable for drinking or irrigation—to cool power plants can reduce freshwater consumption by 94–100%. The results of the study were published in Nature Water.

NETL Publishes New Baseline Study Report on the Flexibility Attributes of Commercial Natural Gas Power Generation Technologies

To address the data needs of energy system designers and to serve as a baseline for research and development, NETL carried out the study "Cost and Performance Baseline for Fossil Energy Plants, Volume 5: Natural Gas Electricity Generating Units for Flexible Operation" to characterize the flexibility attributes—both performance and cost—of nine common commercial natural gas-fueled electricity generating units. According to NETL's Marc Turner, a co-author of the study, "Although existing coal-fired power plants have been increasingly relied upon as loadfollowing resources, current natural gas technologies are much better equipped to follow intermittent renewable generation with faster ramping rates, shorter startup durations, higher efficiency, lower minimum loads, lower water usage, lower costs, and lower emissions. NETL believes this study will provide valuable data as the nation pursues decarbonization goals."

DOE Seeks Information on the Use of Unconventional and Secondary Sources as Feedstocks to Rebuild and Secure a Domestic Critical Minerals Supply Chain

DOE's Office of Fossil Energy and Carbon Management (FECM) released a Request for Information (RFI) that closed July 17, 2023, seeking input on the regional assessment and production of REEs, CMs and novel high-value, nonfuel carbon-based products from unconventional and secondary feedstocks such as coal and coal by-products and effluent waters from oil and natural gas development and production. The input received through the RFI will inform DOE efforts to rebuild the nation's CMs and materials supply chain, which supports high-tech manufacturing and the production of components for clean energy technologies that will help the nation reach the Biden-Harris administration's goal of a net-zero emissions economy by 2050. These efforts will reduce dependence on international supply chains, while also creating good-paying union jobs for American workers and healthier environments for communities across the country.

NETL Researchers Use AI and ML Methods to Design Sorbent That Can Treat Coal Combustion Waste Leachates

Using artificial intelligence (AI) and machine learning (ML) techniques, NETL researchers are exploring a way to treat water that seeps through coal combustion waste using a sorbent synthesized from fly ash, itself a coal combustion waste—a development with implications for improving the costs of managing future waste sites. While investigating the problem of wastewater leaching from coal ash impoundments, NETL researchers realized that AI/ML methods could be used to design sorbents to treat leachates, a liquid pollution that can escape from impoundments. Based on the pore size and composition of the sorbent, zeolites are among the most important sorbents and are frequently used in industrial applications for water and wastewater treatment. NETL researcher Jan Steckel added that the work demonstrates that AI/ML methodologies can be used for rapid, customized sorbent development, greatly reducing the time and expense usually required to develop sorbents for treating impoundment leachates.

Conferences and Events

These upcoming conferences and events align with NETL's water-energy research efforts.

Produced Water Society Permian Basin Summit 2023

Description: This regionally focused technical and business conference brings together 300 water-treatment experts from around the world with regional and global expertise to solve the toughest problems in the produced water field.
 Date: Aug. 14–16, 2023
 Location: Midland, Texas
 Website: https://producedwatersociety.com/event-permian/

The Water Expo

Description: The Water Expo tradeshow is an effective commercial hub to connect manufacturers and distributors with buyers, professionals, dealers, municipalities, contractors and potential representatives from various industries, including wastewater, environmental services, water quality and high pressure and stormwater industries.

Date: Aug. 22–24, 2023 Location: Miami, Florida Website: https://www.thewaterexpo.com/

2023 FECM/NETL Carbon Management Research Project Review Meeting

Description: This meeting will provide attendees with a chance to share in the knowledge and insights gained by more than 150 DOE-sponsored research and development projects from the following FECM research and development programs: Point Source Carbon Capture, Carbon Dioxide Removal, Carbon Conversion and Carbon Transport & Storage.
 Date: Aug. 28–Sep. 1, 2023
 Location: Pittsburgh, Pennsylvania
 Website: https://netl.doe.gov/events/23CM

2023 Annual Forum

Description: The Ground Water Protection Council's 2023 Annual Forum "Looking Back, Moving Forward: 40 Years of Advancing Groundwater Protection and Sustainability" will celebrate an important milestone for the organization.
 Date: Sep. 12–14, 2023
 Location: Tampa, Florida
 Website: https://www.gwpc.org/event/gwpc-annual-forum/

WEFTEC 2023

Description: WEFTEC, "the Water Quality Event," is the world's most comprehensive gathering of water-quality professionals and thought leaders, featuring the sector's leading conference program and a variety of valuable networking opportunities. **Date:** Sep. 30–Oct. 4, 2023

Location: Chicago, Illinois Website: https://www.weftec.org/

WIN Workshop

Description: The WIN (Water treatment Innovation and Networking) Workshop is to provide clients of the Bureau of Reclamation's Brackish Groundwater National Desalination Research Facility (BGNDRF) the opportunity to share their work with a broader audience for networking with potential customers, investors, partners, and other interested parties. **Date:** Oct. 24-25, 2023

Location: Alamogordo, New Mexico Website: https://www.usbr.gov/research/bgndrf/win.html

Researcher Spotlight



Dr. Markus Drouven is a Senior Process Systems Engineer with NETL's Strategic Systems Analysis & Engineering division. Drouven holds a Ph.D. in Process Systems Engineering from Carnegie Mellon University (CMU) and earned both his Bachelor of Science in Mechanical Engineering and Master of Science in Chemical Engineering from RWTH Aachen University in Germany.

After joining NETL in 2020, Drouven is leading DOE's multi-lab, 3-year, \$6 million produced water optimization initiative, "Project PARETO," as the overall Technical Director. The goal of the initiative is to develop, demonstrate and deploy a cutting-edge, optimization-based decision-support framework for oil and gas produced water management and beneficial reuse. He also serves as a Principal Investigator for a task dedicated to leveraging PARETO for REEs and CMs recovery from produced water under the Produced Water Research Partnerships Field Work Proposal. In 2022, Project PARETO won the Hart Energy Meritorious Engineering Innovation Award.

Drouven's research interests include developing and implementing mathematical modeling and optimization solutions for energy systems. He previously worked for EQT Corporation, the largest natural gas producer in the United States, where he was responsible for establishing an in-house optimization engineering team dedicated to leveraging advanced analytics for a broad range of applications including produced water management and development planning.

Recent publications Drouven has co-authored include journal articles titled Mathematical Programming Models for Shale Oil & Gas Development: A Review and Perspective and PARETO: An Open-Source Produced Water Optimization Framework, open source software libraries for Pareto v1.0.0 and WaterTAP v1.0.0, a technical report titled Santa Barbara Desalination Digital Twin Technical Report and presentations on Decision-Making Framework to Evaluate Opportunities for the Recovery of Rare Earth Elements and Critical Minerals in Produced Water Networks for the Produced Water Society Annual Seminar 2023 in Houston, Texas, and on Project PARETO - An Optimization Framework for Produced Water Management and Beneficial Reuse for the September 2021 PARETO Stakeholder Meeting, the 2021 Produced Water Society Seminar, the NAWI Modeling & Simulation Seminar Series, and the University of Texas Permian Basin's 2021 Texas Water and Energy Institute Water Lecture Series.

Water-Energy Publications

Below are several water-related journal articles, reports, and presentations authored or co-authored by NETL staff.

Treatment of brackish water for fossil power plant cooling

Zitao Wu, University of Wyoming; Haibo Zhai, University of Wyoming; Eric Grol, NETL; Chad Able, NETL support contractor; Nick Siefert, (MAY 2023)

https://doi.org/10.1038/s44221-023-00072-x

Application of unsupervised deep learning to image segmentation and in-situ contact angle measurements in a CO₂-water-rock system

Hongsheng Wang, Virginia Tech; Laura Dalton, Duke University; Ruichang Guo, Stevens Institute of Technology; James McClure, Virginia Tech; Dustin Crandall, NETL; Cheng Chen, Stevens Institute of Technology (MARCH 2023) https://doi.org/10.1016/j.advwatres.2023.104385

Effective removal of trace-level toxic metals from flue gas desulfurization wastewater using SiO₂ supported hydrogel sorbent

Qiuming Wang, NETL support contractor; Walter Wilfong, NETL support contractor; Brain Kail, NETL support contractor; Tuo Ji, NETL support contractor; Fan Shi, NETL; McMahan Gray, NETL (MARCH 2023)

https://doi.org/10.1016/j.mtsust.2023.100324

Performance of hydrophobic physical solvents for pre-combustion CO₂ capture at a pilot scale coal gasification facility

Kathryn H. Smith, NETL; Husain E. Ashkanani, Kuwait University; Robert L. Thompson, NETL; Jeffrey T. Culp, NETL; Lei Hong, NETL; Mike Swanson, University of North Dakota; Joshua Stanislowski, University of North Dakota; Wei Shi, NETL; Badie I. Morsi, NETL and University of Pittsburgh; Kevin Resnik, NETL; David P. Hopkinson, NETL; Nicholas S. Siefert, NETL (MARCH 2023)

https://doi.org/10.1016/j.ijggc.2023.103863

'Best' Coal-Fired Power Plant and Cogeneration Case Studies

Stephan Smith, NETL support contractor; Michael Giampetro, NETL support contractor (DECEMBER 2022) https://doi.org/10.2172/1961557

A Decision-Making Framework to Evaluate Opportunities for Recovery of Rare Earth Elements and Critical Minerals in Produced Water Networks

Joshua Pulsipher, CMU; Daniel Ovalle, CMU; Miguel Zamarippa, NETL support contractor; Markus Drouven, NETL; Carl Laird, CMU. Presented at the 2023 Produced Water Society Annual Seminar, Houston, TX (FEBRUARY 2023)

▶ https://netl.doe.gov/energy-analysis/details?id=ef9f50c0-ad88-4aa3-9714-63409fb7bd2d

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> 1450 Queen Avenue SW Albany, OR 97321-2198 541-967-5892

3610 Collins Ferry Road P.O. Box 880 Morgantown, WV 26507-0880 304-285-4764

626 Cochran 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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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 & Tech Transfer Thomas.Feeley@netl.doe.gov 412-779-4115

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



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