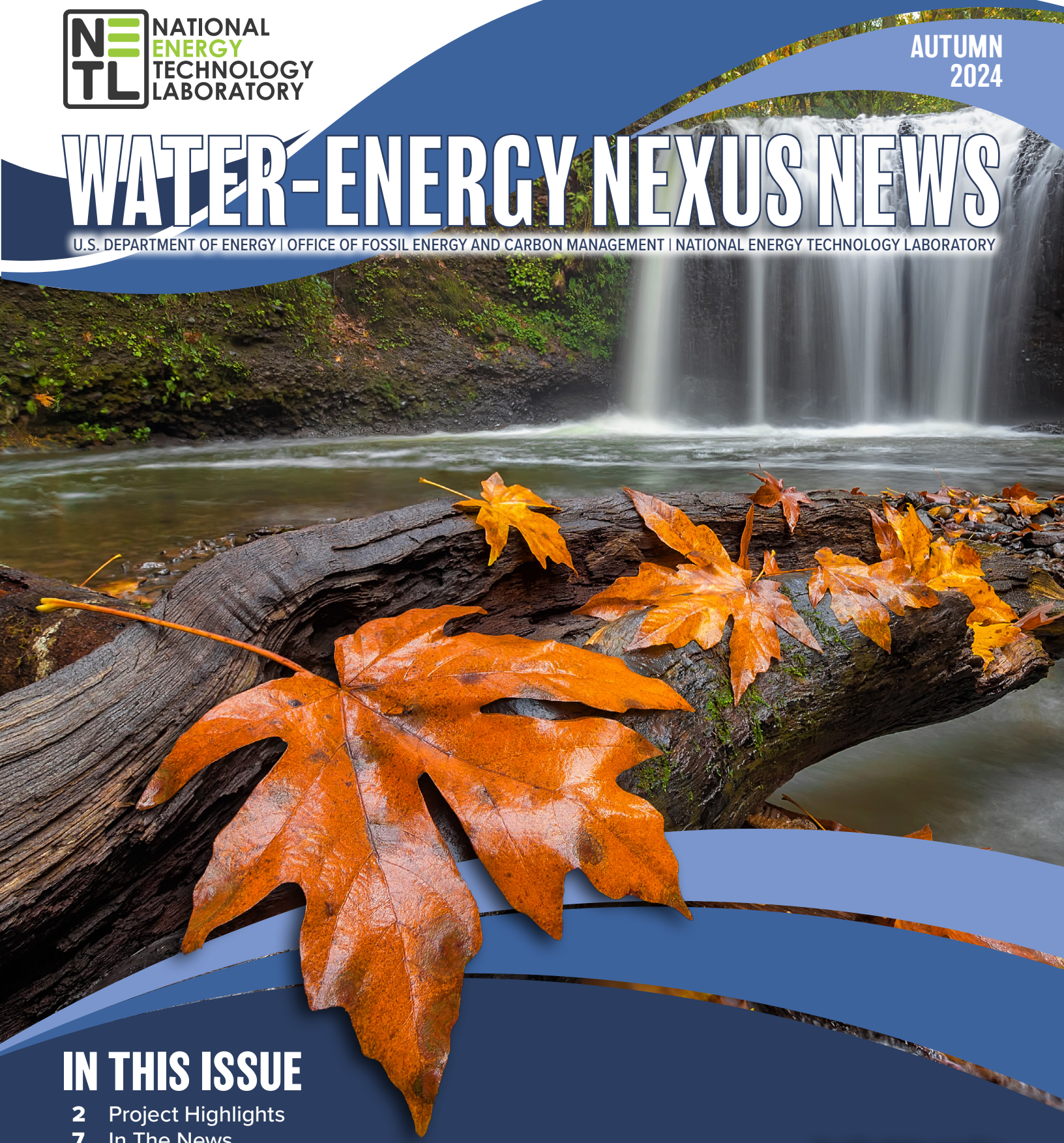
NATIONAL ENERGY TECHNOLOGY LABORATORY

AUTUMN 2024

WATER-ENERGY NEXUS NEWS

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



IN THIS ISSUE

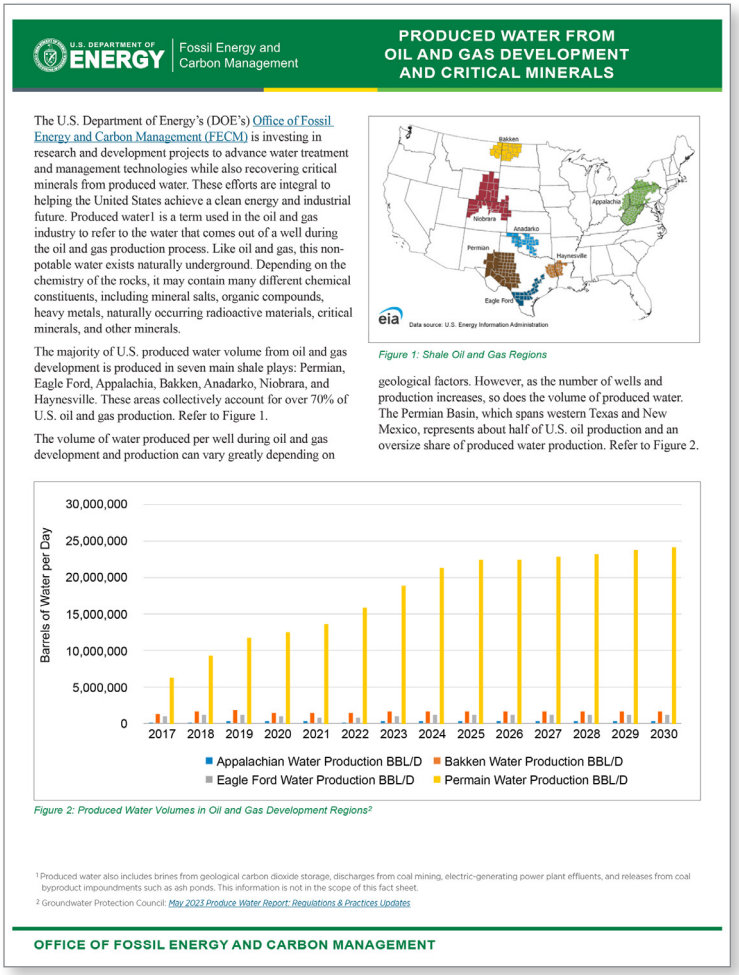
An Update on the National Energy Technology Laboratory's Water-Energy Research and Related Activities

Highlights: New FECM Fact Sheet on Produced Water includes NETL R&D Projects

The Department of Energy's (DOE) Office of Fossil Energy and Carbon Management (FECM) released a new **fact sheet** this summer on produced water and DOE's investment in research and development (R&D) projects to advance water treatment and management technologies while also recovering critical minerals.

Featured projects include NETL R&D work and collaborations such as:

- **Constituent Data Replacement Tool (CoDaRT)**, a tool applying machine-learning approaches for energy wastewater characterization—composition data for CoDaRT can be downloaded from NETL's **National Energy Water Treatment and Speciation Database (NEWTS)** group on Energy Data eXchange (EDX)
- **Produced Water Optimization Initiative (PARETO)**, an open-source, optimization-based, produced water decision-support application
- Water Management Program's Produced Water Research Partnership, a partnership working with universities to develop new capabilities for tools, including machine learning models for NEWTS and PARETO



U.S. DEPARTMENT OF ENERGY | Fossil Energy and Carbon Management

PRODUCED WATER FROM OIL AND GAS DEVELOPMENT AND CRITICAL MINERALS

The U.S. Department of Energy's (DOE's) Office of Fossil Energy and Carbon Management (FECM) is investing in research and development projects to advance water treatment and management technologies while also recovering critical minerals from produced water. These efforts are integral to helping the United States achieve a clean energy and industrial future. Produced water1 is a term used in the oil and gas industry to refer to the water that comes out of a well during the oil and gas production process. Like oil and gas, this non-potable water exists naturally underground. Depending on the chemistry of the rocks, it may contain many different chemical constituents, including mineral salts, organic compounds, heavy metals, naturally occurring radioactive materials, critical minerals, and other minerals.

The majority of U.S. produced water volume from oil and gas development is produced in seven main shale plays: Permian, Eagle Ford, Appalachia, Bakken, Anadarko, Niobrara, and Haynesville. These areas collectively account for over 70% of U.S. oil and gas production. Refer to Figure 1.

The volume of water produced per well during oil and gas development and production can vary greatly depending on geological factors. However, as the number of wells and production increases, so does the volume of produced water. The Permian Basin, which spans western Texas and New Mexico, represents about half of U.S. oil production and an oversize share of produced water production. Refer to Figure 2.

Figure 1: Shale Oil and Gas Regions

Figure 2: Produced Water Volumes in Oil and Gas Development Regions[2]

[1] Produced water also includes brines from geological carbon dioxide storage, discharges from coal mining, electric-generating power plant effluents, and releases from coal byproduct impoundments such as ash ponds. This information is not in the scope of this fact sheet.

[2] Groundwater Protection Council: *May 2023 Produce Water Report: Regulations & Practices Updates*

OFFICE OF FOSSIL ENERGY AND CARBON MANAGEMENT

Highlights: DOE Solicits Applications for FOA to Produce Critical Minerals and Materials; Areas of Interest Include Produced Water

In collaboration with DOE's Office of Energy Efficiency and Renewable Energy, FECM released a funding opportunity announcement (FOA) that will **provide up to $19.5 million** to advance technologies that will help reduce costs for recovering critical minerals and materials from domestic secondary and unconventional sources.

"Advancing Technology Development for Securing a Domestic Supply of Critical Minerals and Materials (CMM)," DE-FOA-0002956, aims to expand programs at FECM and the Advanced Materials and Manufacturing Technologies Office to fund additional processing R&D for the recovery and refining of CMM, as required for critical supply chain use.

The FOA solicits applications in four areas of interest:

- Coproduction of Critical Minerals and Materials and Carbon Manufacturing Precursor Materials from Coal, Coal Waste, and Other Unconventional Carbon-based Feedstocks
- Recovery of Heavy Rare Earth Elements from Secondary and Unconventional Resources
- Critical Mineral Recovery from Produced Water
- Process Diversification: Production of Rare Earth Elements from Secondary/Unconventional Resources and Recycled Materials

Applicants must register with and submit application materials through **NETL eXCHANGE** by the submission deadline, Nov. 26, 2024, at 5:00 PM ET.

Highlights: Conference Proceedings Now Available from FECM/ NETL Carbon Management Review Meeting

Over 150 DOE-sponsored R&D projects were shared at the 2024 FECM/NETL Carbon Management Research Project Review meeting held Aug. 5–9, 2024, in Pittsburgh, Pennsylvania. The annual review meeting recently showcased ongoing work by researchers across the following FECM R&D programs: Point Source Carbon Capture, Carbon Dioxide Removal, Carbon Conversion, and Carbon Transport and Storage.

Some highlights of key presented work at NETL connected to water-energy include the following:

- **Dynamic Reactivity of Mafic Materials due to CO_2 Acidified Brines**, *Dustin Crandall, NETL*
- **Stress Corrosion Cracking of Carbon Steels in CO_2 Pipeline with Water Dropout due to Upset**, *Omer Dogan, NETL*
- **Carbonated Brine Injection Plan**, *Wei Xiong, NETL support contractor*
- **Model-Based Sequential Design of Experiments for Pilot Testing of Novel Water-Lean CO_2 Capture Solvent**, *Lingyan Deng, NETL support contractor*

Full proceedings from the conference are available on NETL's website at **https://netl.doe.gov/24CM-proceedings**

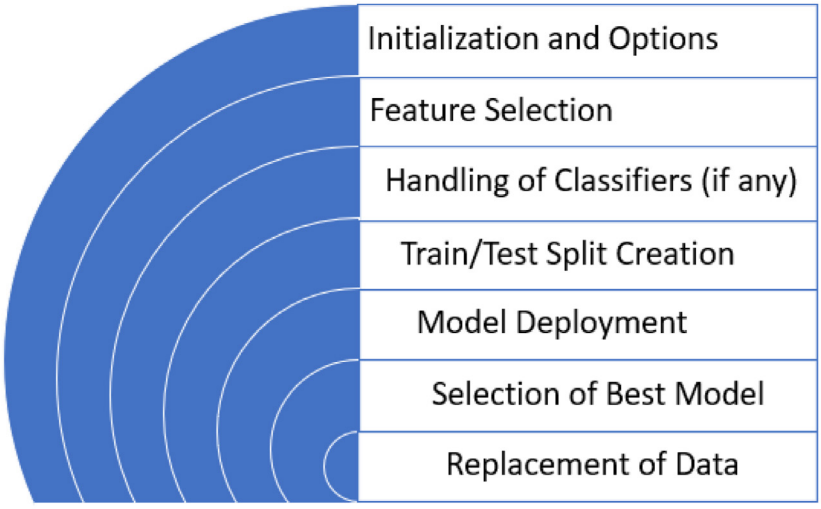
Highlights: A Model Response: CoDaRT Uses Machine Learning to Fill Data Gaps

The U.S. Geological Survey (USGS) maintains approximately 15,000 geochemical profiles in its Produced Water Database. These profiles include such information as the collection location of a wastewater sample, the sample source (whether from coal, shale, sediment or other sources), the acidity or alkalinity of the sample, and the content (minerals, metals, and other substances) of the sample. Some profiles, though, are incomplete. Specifically, many lack data related to rare earth elements (REEs) and critical minerals.

To address these gaps, NETL researchers Dr. Chad Able (support contractor) and Dr. Alison Fritz developed CoDaRT, which uses machine learning to provide missing wastewater data. Machine learning is a subset of artificial intelligence (AI)—it relies on algorithms to imitate how humans learn, consider, and make predictions based on new information. In the case of CoDaRT, machine learning reveals the geochemical trends that arise from a set of samples. Based on those trends, CoDaRT can then predict the makeup of other samples. Effectively, these AI-powered predictions make it possible to complete any sample profile.

When the NETL team devised CoDaRT, they did so with USGS data in mind. They developed the tool, primarily, to replace data missing from the USGS Produced Water Database. The tool, however, can incorporate other water samples as well. It can even combine those samples with existing USGS data to improve the models that influence its predictions.

The conventional approach to understanding wastewater composition entails extensive sampling. The process can be resource-intensive and may still yield incomplete datasets. CoDaRT offers an efficient alternative. Users can tailor the tool to fit their own analyses by selecting various data types, classification features, algorithmic parameters, and other variables. By making these customizations, users can be sure that CoDaRT meets their unique analytical needs—with no additional fieldwork required. The tool operates through a user-friendly interface that allows users to input their data in .csv format. After processing the data, CoDaRT selects the “best fit” models for replacing missing constituents. The output includes vital information, such as constituent concentrations, model performance metrics and computation times, making CoDaRT an invaluable resource for researchers and industry stakeholders alike. Funded by the FECM, the tool is now available on EDX.

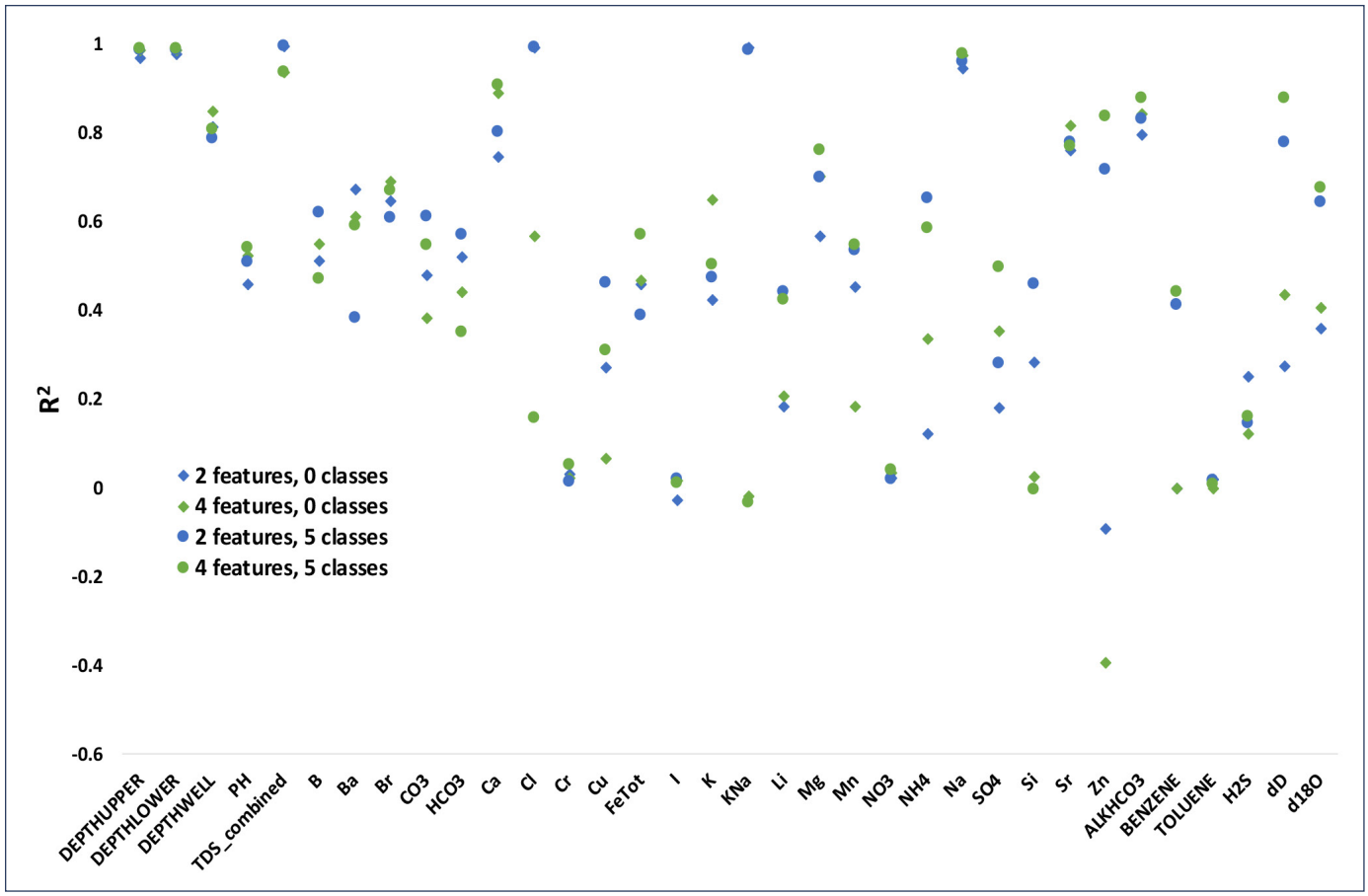


Source: NETL. CoDaRT algorithm overview

(continued)

By providing insights into the composition of coal-ash leachate, hydraulic-fracturing wastewater, and other waste streams, CoDaRT supports the development of wastewater-quality profiles that are comprehensive, correct, and complete. Such profiles are necessary for assessing the treatment needs of particular waste streams. They can also inform the extraction of REEs and critical minerals from wastewater, and they can indicate whether doing so is technologically and economically feasible.

Wastewater streams are auspicious sources of scarce resources. For instance, produced water—a byproduct of hydraulic fracturing—may contain cobalt, lithium, manganese, and nickel, all of which are included on the USGS Critical Minerals List. The United States depends on imports of these materials to manufacture stainless steel, superalloys, and batteries. Pursuing wastewater as a domestic source of these (and other) materials could bolster the supply chains that underlie advanced energy technologies. In this way, CoDaRT exemplifies how NETL's commitment to clean, resilient, and affordable energy is anything but artificial.



Source: NETL. r2 values generated from the sample produced water runs

In the News

NETL Tool That Determines Impact of Energy Production on Water Quality Passes Milestone

NETL's NEWTS Database now contains geochemical, geospatial and other characteristics from more than 400,000 water sample records spanning 48 states, enhancing the ability of the open-source tool to determine the impact of energy production on water quality. The **NEWTS Integrated Dataset** and the **NEWTS State-Level Database Dashboard**, published on EDX, have addressed challenges with finding and using data from collected samples of energy-process water—previously stored in nonstandard formats and managed by various state and federal regulatory agencies—by unifying and standardizing energy-related wastewater data.

NETL Online Tool for Data Discovery Supports Development of Permits for Geologic Carbon Storage

NETL has introduced a free online tool to accelerate the discovery of publicly available data when developing permit applications for the sequestration of CO_2 in the subsurface—the **Carbon Storage Site Mapping Inquiry Tool (MapIT)**. Modules within the tool curate data related to geology, faults, fractures, injection and confining zones, hydrologic information, groundwater, groundwater wells, geomechanical and petrophysical data and geochemical data.

NETL, Partners Report Breakthrough Research Results to Advance Geothermal Technology

The successful completion of field operations by researchers at the Utah Frontier Observatory for Research in Geothermal Energy, also known as the Utah FORGE, and supported by NETL represents a significant step forward to advance geothermal energy as a resource that will produce renewable clean electricity for the nation's power grid.

NETL Carbon Mineralization Article Highlights Lab's Achievements in Research Field

NETL's work in developing carbon mineralization technologies, which presents an alternative pathway toward a decarbonized power sector and economy, is gaining widespread recognition from the greater research community. Natural resources for carbon mineralization include natural brines and mafic/ultramafic rocks and minerals. These types of carbon mineralization processes offer a means to store CO_2 in various geologic settings, including within significant basalt formations. An **article** co-authored by NETL experts is among the most read articles and the most cited articles published in *ChemBioEng Reviews*.

Conferences and Events

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

The International Water Conference® (IWC)

Description: The IWC is a robust educational conference, founded with an emphasis on commercial-free discussions on technology. It is dedicated to advancing new developments in the treatment, use and reuse of water for industrial and other engineering purposes.
Date: Nov. 3–7, 2024
Location: Las Vegas, Nevada
Website: https://eswp.com/water/overview/

Society of Petroleum Engineers (SPE) Workshop: Full Life Cycle Management of Produced Water

Description: This SPE workshop features interactive sessions led by experts in the field, covering topics such as current regulatory frameworks, volume reduction strategies, best practices in offshore produced water management, cutting-edge treatment technologies, sustainable beneficial reuse strategies and mineral extraction from produced water.
Date: Nov. 19–20, 2024
Location: Galveston, Texas
Website: https://www.spe-events.org/workshop/full-life-cycle-management-of-produced-water

2024 Association of California Water Agencies (ACWA) Fall Conference & Expo

Description: ACWA conferences are the premier destination for water industry professionals to learn and connect. New programming will showcase case-study presentations, product demonstrations or other dynamic looks at how others in the industry are addressing today's challenges.
Date: Dec. 3–8, 2024
Location: Palm Desert, California
Website: https://www.acwa.com/events/2024-fall-conference-expo/

Produced Water Society 35th Annual Conference

Description: The Produced Water Society's annual conference brings together experts to discuss the technological advancements of produced water management and treatment across multiple topics.
Date: Feb. 10–13, 2025
Location: Houston, Texas
Website: https://producedwatersociety.com/event-pws-35th-annual-conference/

Researcher Spotlight

Justin Mackey

Research Geochemist

justin.mackey@netl.doe.gov

Justin Mackey is a site-support contractor assisting NETL's Geochemistry team. He earned his master's degree in Geology and Environmental Science from the University of Pittsburgh in 2017 and his bachelor's degree in Geological and Earth Sciences/Geosciences from Northeastern Illinois University in 2012. Mackey is currently a Ph.D. candidate at University of Pittsburgh in the Department of Geology and Environmental Sciences.

Mackey joined NETL over six years ago as an Oak Ridge Institute for Science and Education (ORISE) research associate before moving over in 2020 to support NETL as a research geochemist through Leidos. His current research thrusts focus on locating and characterizing critical mineral resources from unconventional ores, developing novel methods to monitor the environmental impacts of aging energy infrastructure and finding novel solutions to remediate fossil energy wastes (emissions and fluids).

Mackey's research centers on creating solutions to fundamental problems in the mining and energy industries. He is lead investigator of a project developing deposit and source attribution models for lithium and other critical minerals from produced water generated during onshore oil and gas operations. Mackey is an active contributor to the Pittsburgh Water Collaboratory and organizes the Produced Water Working Group meeting at NETL to facilitate discussions and synergies between researchers and stakeholders working in the produced water/critical minerals space. Additionally, Mackey supports ongoing efforts for the NEWTS Database and Carbon Mineralization projects.

Recent publications Mackey has co-authored include journal articles—**Critical mineral source potential from oil & gas produced waters in the United States** and **Estimates of lithium mass yields from produced water sourced from the Devonian-aged Marcellus Shale**—and presentations **Characterizing Radium Distributions, Source Attribution and Impacts from Marcellus Produced Water**, **Estimating Lithium Fluxes from Produced Water: Marcellus Shale and Beyond**, **National Energy Water Treatment & Speciation (NEWTS): A Water & Critical Mineral Database and Dashboard** and **Predicting Lithium Fluxes from a Heterogenous Brine Source: Marcellus Shale**.

Publications and Presentations

Below are several water-related publications and presentations authored or co-authored by NETL staff.

Estimates of lithium mass yields from produced water sourced from the Devonian-aged Marcellus Shale

Justin Mackey, NETL support contractor; Daniel Bain, NETL; Greg Lackey, NETL; James Gardiner, NETL; Djuna Gulliver, NETL; Barbara Kutchko, NETL. (APRIL 2024)

▸ https://doi.org/10.1038/s41598-024-58887-x

Computed Tomography Scanning and Geophysical Measurements of UW Enterprises LP 1-250512-129 Well in Southwestern Indiana

Lianbo Hu, NETL support contractor; Thomas Paronish, NETL support contractor; Dustin Crandall, NETL; Karl Jarvis, NETL support contractor; Natalie Mitchell, NETL support contractor; Sarah Brown, NETL support contractor; Scott Workman, NETL support contractor; Ashley Douds, Indiana University; Maria Mastalerz, Indiana University. (JUNE 2024)

▸ https://netl.doe.gov/energy-analysis/details?id=f744cef9-f671-41aa-953a-0240baf28721

Critical mineral source potential from oil & gas produced waters in the United States

Kathryn Smith, NETL; Justin Mackey, NETL support contractor; Madison Wenzlick, NETL; Burt Thomas, NETL; Nicholas Siefert, NETL. (JUNE 2024)

▸ https://doi.org/10.1016/j.scitotenv.2024.172573

Impacts of irregularly-distributed acidified brine flow on geo-chemo-mechanical alteration in an artificial shale fracture under differential stress

Samantha Fuchs, University of Texas at Austin (UT Austin); Dustin Crandall, NETL; Johnathan E. Moore, NETL; Mayandi Sivaguru, University of Illinois; Bruce Fouke, University of Illinois; D. Nicolas Espinoza, UT Austin; Ange-Therese Akono, Northwestern University; Charles J. Werth, UT Austin. (MAY 2024)

▸ https://doi.org/10.1016/j.ijggc.2024.104127

Utica/Point Pleasant brine isotopic compositions (δ7Li, δ11B, δ138Ba) elucidate mechanisms of lithium enrichment in the Appalachian Basin

Bonnie McDevitt, USGS; Travis L. Tasker, Saint Francis University; Rachel Coyte, New Mexico Institute of Mining and Technology; Madalyn S. Blondes, USGS; Brian W. Stewart, University of Pittsburgh; Rosemary C. Capo, University of Pittsburgh; J. Alexandra Hakala, NETL; Avner Vengosh, Duke University; William D. Burgos, Pennsylvania State University; Nathaniel R. Warner, Pennsylvania State University. (OCTOBER 2024)

▸ https://doi.org/10.1016/j.scitotenv.2024.174588

Modeling and Optimization of Zeolites for Contaminant Removal from Coal Combustion Impoundment Leachates

John Findley, NETL support contractor; Eric Grol, NETL; Evan Granite, NETL; Janice Steckel, NETL. (JUNE 2024)

▸ https://netl.doe.gov/energy-analysis/details?id=8547105a-556b-40ff-a3ed-6ae63e49296c

NAWI Research Spotlight: Technoeconomic Assessment of Brine Valorization from Brackish Groundwater

Alison Fritz, NETL; Casey Finnerty, Yale University; Alexander Dudchenko, SLAC National Accelerator Laboratory; Haleigh Heil, NETL support contractor; Caroline Adkins, Stanford University; Meagan Mauter, Stanford University; Adam Atia, NETL support contractor; Chad Able, NETL support contractor; Erik Shuster, NETL. (June 2024)

▸ https://netl.doe.gov/energy-analysis/details?id=b3e3c37a-78e7-440e-bd84-d89afd619105

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:

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Contact Us

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

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