USGS
science for a changing world

Quarter 1, 2024

Issue #13

Front & Center!

Quarterly Science Newsletter

Frontline Science within the Geology, Energy & Minerals (GEM) Science Center, Reston, Virginia

Center Director Note

Welcome to the thirteenth issue of the USGS Geology, Energy & Minerals Science Center (GEM or GEMSC) quarterly newsletter. The dedication and hard work of our GEM teams has truly been remarkable and productive, with some impactful publications and products being released. Since the last issue, GEM staff have released 12 professional manuscripts, 11 scientific data releases, and have presented at several scientific meetings or conferences around the world. We also are advertising several new positions (*see page 4 for more information*).

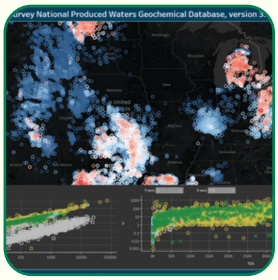
I am thrilled to witness the remarkable growth of interdisciplinary collaboration within our Science Center. The installation of our new microprobe and automated mineral analyzer represents a significant milestone in our pursuit of cutting-edge research. These advanced tools not only enhance our capabilities but also signify our commitment to exploring new frontiers in science. With these additions, we are poised to delve deeper into the realms of energy transition, critical minerals, and the utilization of energy and mineral waste and byproducts as a resource for rare earth elements and critical minerals. By conducting comprehensive research in this area, the USGS can contribute valuable insights that may shape the future of energy production and consumption. Furthermore, our exploration of critical minerals underscores our dedication to addressing pressing global challenges. As demand for these resources continues to rise, it is imperative that we understand their significance and explore innovative ways to ensure their availability for future generations. Additionally, our investigation into energy and mineral waste as a potential resource for rare earth elements and minerals exemplifies our commitment to sustainability. By reimagining waste products as valuable commodities, we not only evaluate ways to mitigate environmental impact but also unlock new avenues for resource utilization. Through our research on studying the environmental impacts of energy and mineral development, we aim to inform policy decisions and industry practices to minimize harm in the environment and promote sustainability.

If you have any comments, questions, or ideas for collaboration, please reach out to me directly (troberts-ashby@usgs.gov). To explore more about what we do in our Science Center, please visit our USGS GEMSC website. If you know anyone who may be interested in receiving this newsletter, or if you would like to adjust your subscription status, please refer to the online subscription form.

~ Tina Roberts-Ashby Ph.D., GEM Science Center Director

Science Spotlight

U.S. Geological Survey National Produced Waters Geochemical Database (ver. 3.0, December 2023)



Snapshot image from Blondes et al., 2023, USGS Produced Waters Geochemical Database (ver. 3.0, December 2023).

During hydrocarbon production, water is typically co-produced from the geologic formations producing oil and gas. Understanding the composition of these produced waters is important to help investigate the regional hydrogeology, the source of the water, the efficacy of water treatment and disposal plans, potential economic benefits of mineral commodities in the fluids, and the safety of drinking or agricultural water. In addition to waters co-produced with hydrocarbons, geothermal development or exploration brings deep formation waters to the surface for possible sampling. The U.S. Geological Survey (USGS) Produced Waters Geochemical Database (ver. 3.0, December 2023), which contains geochemical and other information for produced water and other deep formation water samples of the United States, is an updated version of the USGS Produced Waters Database (Blondes and others, 2019). The purpose of the database is to provide background information on the composition of waters produced along with oil and gas to relevant stakeholders, including industry, the government, environmental groups, and the public.

Scanning Electron Microscope (SEM) images of selected age-diagnostic foraminifera found in sediments from the Nuwok Member at 1075 Carter Creek, from Figure 6 in 'Insights into glendonite formation from the upper Oligocene Sagavanirktok Formation, North Slope, Alaska', *International Journal of Sedimantary Research*, courtesy of John Counts, Research Geologist, USGS, 2023.

Science Spotlight (Continued)

Illegal Dumping of Oil and Gas Wastewaters Alters Arid Soil Microbial Communities

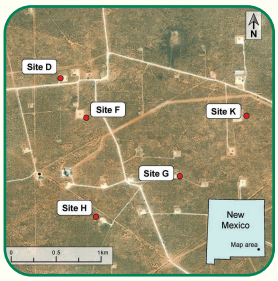


Figure 1 from Kashani et al., 2024 in Applied Environmental Microbiology.

Scientists from the GEMSC, USGS Water Resources Mission Area, USGS Maryland-Deleware-District of Columbia Water Science Center, University of Texas at El Paso, and Bureau of Land Management published a manuscript in *Applied and Environmental Microbiology* that describes the effects of unpermitted releases of oil and gas (OG) wastewater on arid soil geochemistry and microbial communities in southeastern New Mexico. They analyzed changes in soil geochemistry and microbial community composition by comparing soils from within OG wastewater dump-affected zones to corresponding unaffected (control) zones. They observed significant changes in soil geochemistry for all dump-affected samples compared to controls, reflecting the residual salts and hydrocarbons left behind by the OG wastewater release (e.g., enriched in sodium (Na), chloride (Cl), and bromide (Br)). Microbial communities in OG wastewater-affected soils had significantly lower diversity and differences in phylogenetic composition. OG wastewater-affected soils showed an increase in salt-tolerant organisms suggesting that the high salinity of the OG wastewater was a strong selective pressure for microbial communities. Taxa with capabilities to metabolize hydrocarbons were also detected in the OG wastewater-affected soil communities. Overall, this study revealed changes in arid soil geochemistry and microbial community dynamics due to OG wastewater exposure.

Using Stochastic Point Pattern Analysis to Track Regional Orientations of Magmatism During the Transition to Cenozoic Extension and Rio Grande Rifting, Southern Rocky Mountains

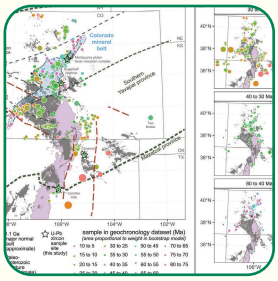
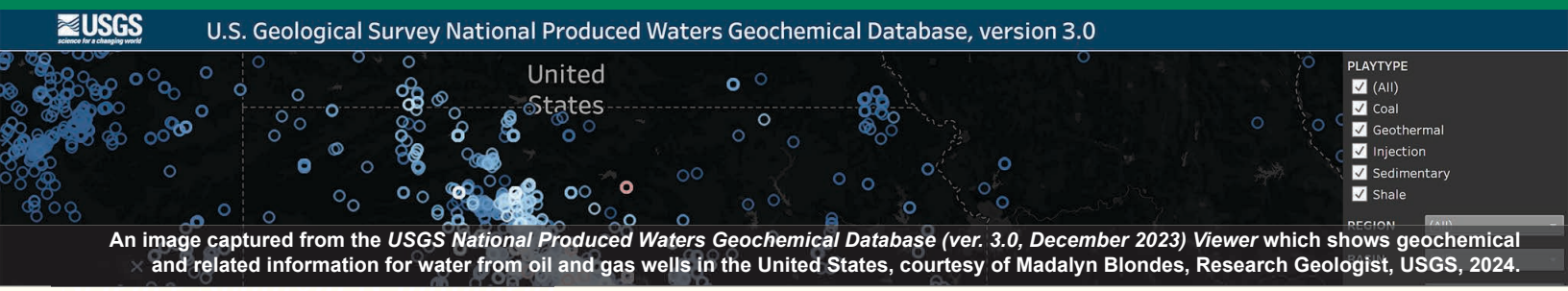


Figure 1 from Rosera et al., 2024 in Tectonics.

GEMSC Staff and collaborators from Princeton University, the University of Lausanne, and the University of Geneva published new research about modeling spatial patterns of magmatism. This new method attempts to reduce biases that come with geochronological datasets built from a variety of sources. The study focuses on magmatism in the southern Rocky Mountains but may broadly be of interest to geologist who wish to understand or model spatial-temporal patterns of magmatism in other regions. This work is a step towards 1) using explicit analytical tools to map magmatism, rather than relying on hand-drawn features, and 2) generating more reproducible results with scripts that accompany the research. Generating reproducible spatial models for magmas is useful for geological mapping, modeling, and understanding distributions of certain magma-related mineral deposits.



An image captured from the *USGS National Produced Waters Geochemical Database (ver. 3.0, December 2023) Viewer* which shows geochemical and related information for water from oil and gas wells in the United States, courtesy of Madalyn Blondes, Research Geologist, USGS, 2024.

Science Spotlight (Continued)

A New Quick Screening Tool for Approximating Rare Earth Elements (Q-STAR) in Natural Waters

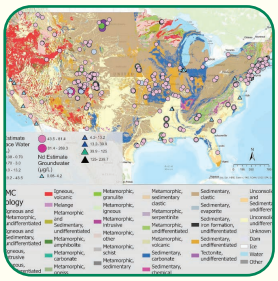
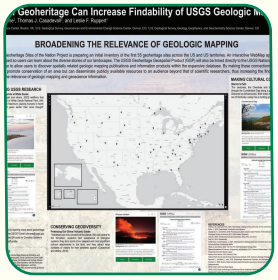


Figure 3 from Tomaszewski et al., 2024 in Journal of Geochemical Exploration.

GEMSC Research Chemist Beth Tomaszewski, in collaboration with the Army Corps of Engineers, developed a new method to rapidly screen natural water samples for the presence of rare earth elements (REEs). REEs are a class of critical minerals which have supply chain vulnerabilities that can impact economic security. These elements are widely measured by inductively coupled plasma mass spectrometry (ICP-MS); however, this approach can be time consuming and costly. This new Quick Screening Tool for Approximating REEs (Q-STAR) can detect REEs in surface water and groundwater samples. A mass-to-charge ratio of 144 (m/z = 144) was added to an ICP-MS method to screen for REEs in filtered water samples submitted for metals analyses to the U.S. Geological Survey National Water Quality Laboratory. REEs were detected above a reference threshold of 1200 counts per second in 18% of pre-selected 6626 samples. Using this screened dataset, estimated REE concentrations were mapped across the United States in relation to ecoregions and underlying geology. Q-STAR can be used to screen an unlimited number of water samples for the presence of REEs prior to time-intensive and costly quantitative analyses and to generate large REE datasets for further investigation.

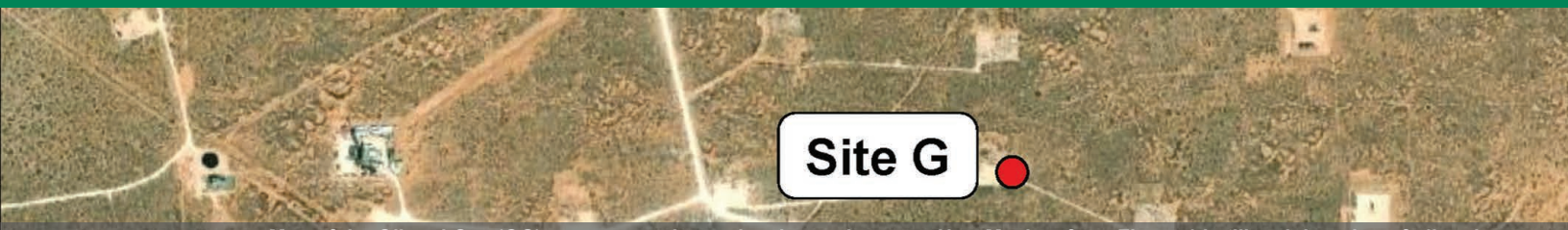
How the Concept of Geoheritage Can Increase Findability of USGS Geologic Mapping Products



Poster from DeVera et al., 2023, prepared for the American Geophysical Union Annual Meeting, December 11-15, 2023, San Francisco, CA.

GEMSC Physical Scientist, Christina DeVera, presented a poster, at the *American Geophysical Union (AGU) Conference 2023* in San Francisco, CA on December 14th, 2023 during the poster session, *Understanding the Societal Value and Use of Earth Science Information II*. This poster outlines how the National Cooperative Geologic Mapping Program geoheritage geospatial product (GGP) will provide an educational and outreach tool to raise awareness of significant geologic sites, communicate the role of geology in our natural heritage, and make geologic mapping and geoscience topics more accessible and relevant to the public. Connecting geoheritage values to scientifically significant geologic features can create access points for the discovery of USGS geologic mapping, information products, and data enabling the public to better understand the landforms and their related geologic processes. The GGP will also be linked directly to the USGS National Geologic Map Database to allow users to discover spatially related geologic mapping publications and information products within the expansive database. By making these

(continued on page 4)



Map of the Oil and Gas (OG)-wastewater dump sites in southeastern New Mexico, from Figure 1 in 'Illegal dumping of oil and gas wastewater alters arid soil microbial communities', *Environmental Microbiology*, courtesy of Isabelle Cozzarelli, Research Hydrologist, USGS, 2024.

Science Spotlight (Continued)

(continued from page 3)

connections, the GGP not only has the potential to inform land management decisions of an area but can disseminate publicly available resources to an audience beyond that of scientific researchers, thus increasing the discoverability and broadening the relevance of geologic mapping and geoscience information.

For more information contact Christina DeVera (cdevera@usgs.gov)

Employee Corner

Sylvia Hasley-Velez (Willow)

Willow joins GEMSC as an intern with the USGS Pathways Internship Program. She received her B.S. in Earth Science with a concentration in Geology at George Mason University and is continuing her education through the same university with a M.S. in Earth System Sciences. Her thesis focuses on the behavior of the U-isotope proxy under varying suboxic to anoxic, non-euxinic, conditions in modern settings. In her free time, she enjoys hiking, cooking, and crocheting.

Join Our Team! ~ Job Opportunities

The GEMSC frequently has opportunities for bringing in new staff. We are preparing advertisments for the following positions:

- Geologist, GS-9/11
- Physical Scientist Technician, GS 7/9/11 - Safety/Records Management

These vacancies, as well as future GEMSC vacancies, are advertised on USAJobs and will appear in USAJobs before they appear in our newsletter. Stay tuned to this section for news on future job opportunities with GEMSC.

Photograph montage of Aaron Jubb, Research Chemist, USGS working in laboratory and field settings, and climbing in Great Falls Park. Background is a montage of white light, fluorescence, SEM, cathodoluminescence, and photothermal images from a source rock field of view.

Scientist Profile ~ Aaron Jubb

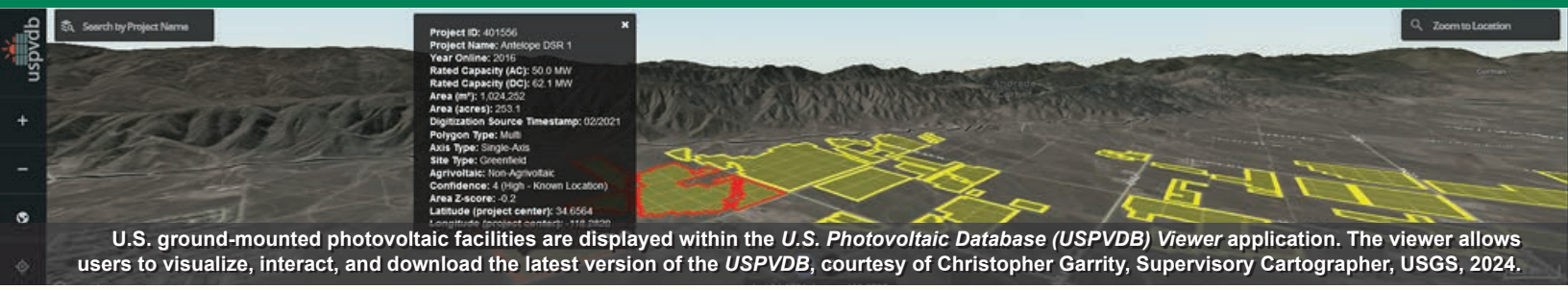
I am a research chemist in the Geology, Energy & Minerals Science Center and have worked at the U.S. Geological Survey (USGS) since January 2017. My path to the USGS working on energy resources could be considered "non-traditional" when compared to most of my colleagues. I received a Ph.D. in Analytical Chemistry from The Ohio State University in 2012 working with Professor Heather Allen on fundamental science topics relevant to interfacial atmospheric and geochemical processes. For example, the structure of water molecules at the air-water interface, with roughly 2 hydrogen bonds each, is very different than water molecules in bulk solution where each water molecule has ~3.5 hydrogen bonds. Such phenomena impact a suite of physical and chemical processes ranging from atmospheric aerosol growth to adsorption of ions at mineral surfaces. To study these types of systems I employed a non-linear vibrational spectroscopy called vibrational sum frequency generation (VSFG). VSFG provides signal only from molecules lacking an inversion center allowing for discrimination of surface signals from much larger signals given by bulk volumes. VSFG is not for the faint of heart; think (i) big lasers, (ii) dark, cold rooms, and (iii) long hours.

Aaron Jubb, Research Chemist, USGS GEMSC.

Following my Ph.D., I was fortunate to be able to pursue a post-doctoral appointment at the National Oceanic and Atmospheric Administration (NOAA) laboratory in Boulder, Colorado. At NOAA my research focused on atmospheric chemical kinetics of halogenated industrial chemicals (e.g., tetrafluoroethane, the primary refrigerant in automobile air conditioners). This position broadened my scientific toolkit by exposing me to kinetic methods as well as what it was like to work in a federal research center. It was also great to work in a laboratory where the lights could be turned on. Additionally, living in Boulder, with the Flatirons as a playground, was really fun. My experience at NOAA clarified that I desired a career as a federal researcher, as opposed to a academic or industrial position. So, when my time at NOAA ended, I was off to Knoxville, Tennessee to work in Dr. Baohua Gu's group at Oak Ridge National Laboratory (ORNL). My work at ORNL differed (again) from my previous research and revolved around the design and fabrication of surface enhanced Raman (SERS) sensors for field-based perchlorate detection in groundwater. Baohua was an excellent mentor and supervisor, he provided ample resources to his group and then got out of the way! I often think of Baohua's example of trusting his employees to do a good job without micromanaging their day-to-day as I negotiate my own supervisory responsibilities.

In 2017 I had the opportunity to come to the USGS in Reston, Virginia to work in what was then known as the Eastern Energy Resources Science Center. I was hired by Leslie "Jingle" Ruppert, who was a fantastic supervisor and is a continuing inspiration to me. My USGS work started primarily in a laboratory management role as energy-funded laboratories were fully implementing the new quality management system (QMS) in 2017. Once QMS issues were sorted, I transitioned to a primary research role where my work focuses on three topics; (i) sedimentary organic matter structure-reactivity relationships, (ii) porosity and fluid behavior in geologic matrices and (iii) oil and gas-associated wastewaters. Toward these ends I currently lead the Energy Resources Program (ERP)-funded Advancements in Geochemistry and Geomicrobiology of Energy Resources (AGGER) project and participate as a task lead on the ERP-funded Oil and Gas Waters project. Once again, these topics are outside of my formal training. From my experiences bouncing around various research topics over the past 10+ years, I think an important lesson is that your value as a researcher is more than your current expertise. It is the ability to bring creative solutions to bear on important problems that is truly valuable.

Finally, a word about non-professional pursuits. My partner and I live in Reston, Virginia where we have a very wiggly 2-year old son. We enjoy the Reston trails and generally getting outside. My son adds that elephants are his favorite. I also greatly enjoy rock climbing. While the mid-Atlantic region is not known for rock climbing locales, there are excellent opportunities for close-to-home exploration around Great Falls Park on the banks of the Potomac. This was a real life saver for me during the pandemic and continues to be a favorite post-work destination.



U.S. ground-mounted photovoltaic facilities are displayed within the *U.S. Photovoltaic Database (USPVDB) Viewer* application. The viewer allows users to visualize, interact, and download the latest version of the *USPVDB*, courtesy of Christopher Garrity, Supervisory Cartographer, USGS, 2024.

Quarter 1 Publications and Data Releases by GEMSC Authors

Publications (USGS and External)

Cathodoluminescence Differentiates Sedimentary Organic Matter Types: https://www.nature.com/articles/s41598-024-53168-z

Chemical Composition of Leachates from Hydraulic Fracturing Proppants from Surficial Releases in Southeastern New Mexico: https://doi.org/10.1021/acs.estlett.3c00911

Comparison of Measured Versus Modeled TOC in the Tuscaloosa Marine Shale of Southwestern Mississippi, U.S.A.: https://doi.org/10.1016/j.marpetgeo.2023.106655

Defining the Hafnium Isotopic Signature of the Appalachian Orogen Through Analysis of Detrital Zircons from Modern fluvial Sediments: https://doi.org/10.1086/730281

Deformation Induced Graphitization and Muscovite Recrystallization in a Ductile Fault Zone: https://doi.org/10.1111/jmg.12763

Insights into Glendonite Formation from the Upper Oligocene Sagavanirktok Formation, North Slope, Alaska: https://doi.org/10.2110/jsr.2023.060

Non-Mercury Methylating Microbial Taxa are Integral to Understanding Links Between Mercury Methylation and Elemental Cycles in Marine and Freshwater Sediments: https://doi.org/10.1016/j.envpol.2024.123573

Novel Insights About Petroleum Systems from Source and Reservoir Rock Characterization, Cretaceous Deposits, Babouri-Figuil Basin, Northern Cameroon: https://doi.org/10.1016/j.coal.2024.104491

Spatial Distribution of API Gravity and Gas/Oil Ratios for Petroleum Accumulations in Upper Cretaceous Strata of the San Miguel, Olmos, and Escondido Formations of the South Texas Maverick Basin—Implications for Petroleum Migration and Charge History: https://doi.org/10.3133/sir20235124

The Addition of 144Nd to Routine ICP-MS Analysis as a Quick Screening Tool for Approximating Rare Earth Elements (Q-STAR) in Natural Waters: https://doi.org/10.1016/j.gexplo.2024.107401

Uranium Redox and Deposition Transitions Embedded in Deep-Time Geochemical Models and Mineral Chemistry Networks: https://doi.org/10.1029/2023GC011267

Using Stochastic Point Pattern Analysis to Track Regional Orientations of Magmatism During the Transition to Cenozoic Extension and Rio Grande Rifting, Southern Rocky Mountains: https://doi.org/10.1029/2023TC007902

USGS Data Releases

Chemistry Data from Leachates of Hydraulic Fracturing Proppants Collected from Southeastern New Mexico, 2018-2019: https://doi.org/10.5066/P90KK04S

Data from Cretaceous Formations of the Babouri-Figuil Sedimentary Basin, Northern Cameroon: https://doi.org/10.5066/P9N1CDFW

Database of Mineral Deposits Related to the Mesoproterozoic Midcontinent Rift System (MRS) in the Northern United States and Northern Ontario, Canada: https://doi.org/10.5066/P9HTATKY

Delta Log R Total Organic Carbon Estimates for the Tuscaloosa Marine Shale, U.S.A.: https://doi.org/10.5066/P91KVUN1

Detrital Zircon U-Pb and Hf Isotope Data from Selected Appalachian Rivers: https://doi.org/10.5066/P9XP68PG

National Scale Assessment for Rare Earth Elements in Dissolved Water Samples and Supporting Geochemistry: https://doi.org/10.5066/P95TDKA4

Screening Geochemistry, Gas Chromatography, and Solid Bitumen Reflectance Data in the Bakken Petroleum System, Williston Basin, USA: https://doi.org/10.5066/P9R5PQFN

United States Large-Scale Solar Photovoltaic Database (ver. 1.0, November 2023): https://doi.org/10.5066/P9IA3TU

United States Gulf Coast Basin Curated Wells and Logs Database (ver. 2.0, November 2023): https://doi.org/10.5066/P95BNWT3

United States Wind Turbine Database (ver. 6.1, November 2023): https://doi.org/10.5066/F7TX3DN0

U.S. Geological Survey National Produced Waters Geochemical Database (ver. 3.0, December 2023): https://doi.org/10.5066/P9DSRCZJ