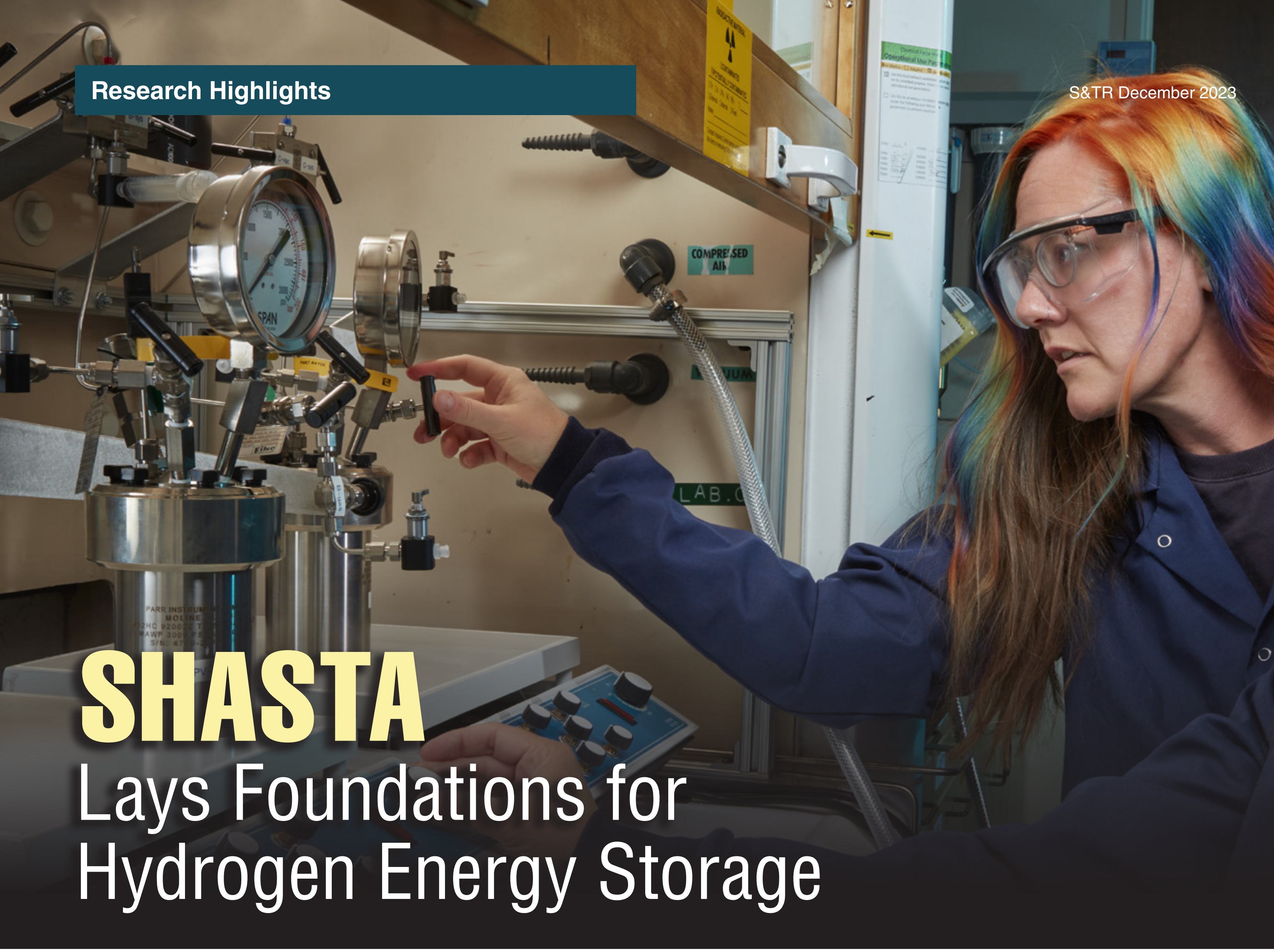


SHASTA Lays Foundations for Hydrogen Energy Storage

THE universe's lightest molecule may have massive implications for the nation's climate and energy security. Abundant and non-polluting, hydrogen gas could help meet growing domestic energy demand while spurring a low-carbon economy and reinforcing energy reliability, diversification, and independence. When renewable energy sources such as wind and solar generate more supply than demand requires, the surplus, stored as chemical energy in hydrogen, could ensure a retrievable electricity source decoupled from fluctuations in energy production and seasonal shifts in utilization.

Adopting emerging technologies is easier said than done. Questions remain before hydrogen storage can be widely integrated with the energy grid. To tackle knowledge gaps, the Department of Energy (DOE) Office of Fossil Energy and Carbon Management launched the Subsurface Hydrogen Assessment, Storage, and Technology Acceleration (SHASTA) project in 2021. Carried out jointly by Lawrence Livermore, Sandia, and Pacific Northwest national laboratories and the National Energy Technology Laboratory, SHASTA addresses the intricacies of maintaining hydrogen fuel reserves.

Chemical Potential

Joshua White, deputy division leader for Science & Technology in the Atmospheric, Earth, and Energy Division and Livermore's technical lead for SHASTA, explains the growing interest in hydrogen energy: "The difficulty with electricity generation is that you must either use the energy immediately or store it. Typically, the term 'energy storage' brings to mind batteries in phones or electric vehicles that are drained and recharged daily. Hydrogen, by contrast, is meant to address industrial-scale energy storage on the order of months or years." Extensive research efforts underway address production, transport, and use of hydrogen fuel. SHASTA targets the foundation. "A crucial challenge is reliably storing hydrogen at scale in the first place," says White.

For solutions, researchers are digging deep. Naturally occurring, underground reservoirs make attractive locations thanks to their enormous volume and intrinsic layers of security. These vast subterranean voids could safeguard nearly 10 million metric tons of storage of pure hydrogen—an energy potential of more than 300 terawatt-hours. Depleted hydrocarbon fields are particularly promising candidates. These fields are abundant and

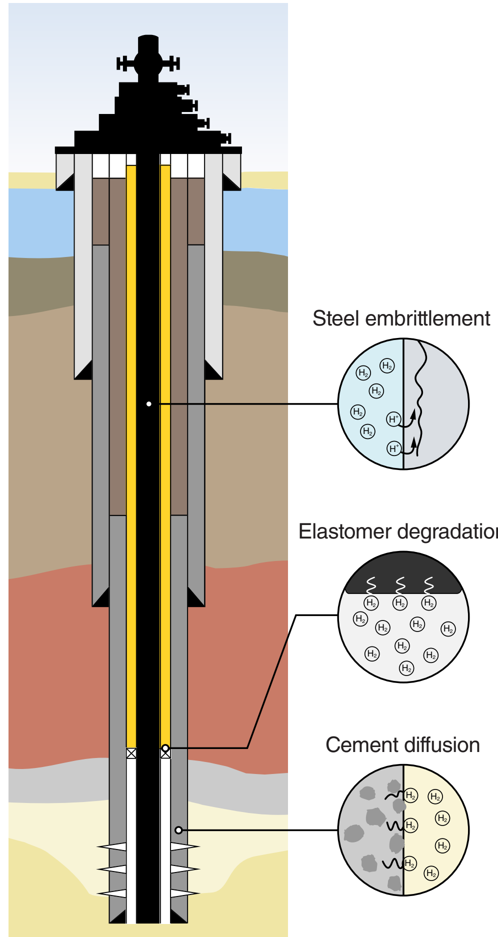
Researchers Megan Smith (left) and Maria Gabriela Davila-Ordonez (right) demonstrate the new experimental setup for testing the response of geologic and well infrastructure materials to heightened hydrogen concentration. Stainless steel vessels hold material coupons at representative pressure and temperature conditions for up to one month, and periodic fluid samples complement post-assay inspection to determine chemical or physical changes.

capable of holding fluid mixtures, as evidenced by existing well infrastructure from earlier oil and natural gas extraction. Other contenders such as salt caverns and saline aquifers offer unique advantages and challenges.

What remains unresolved is how best to maximize the safety and cost-effectiveness of underground hydrogen storage (UHS). In 2022, the program's State of Knowledge report detailed new findings and outstanding questions—notably, the numerous physical, chemical, and even biological interactions that could result from introducing hydrogen into reservoirs, possibly impacting storage efficiency and well integrity. Moreover, no two reservoirs are identical, nor are they distributed evenly across the continental United States, meaning SHASTA must address both scientific and technoeconomic aspects of UHS.

The Pressure Is On

Residing kilometers below Earth's surface, candidate reservoirs cannot be observed directly. Determining suitability for UHS demands scientific methods to recreate subterranean environments in the laboratory. Of primary concern is assessing the capability of

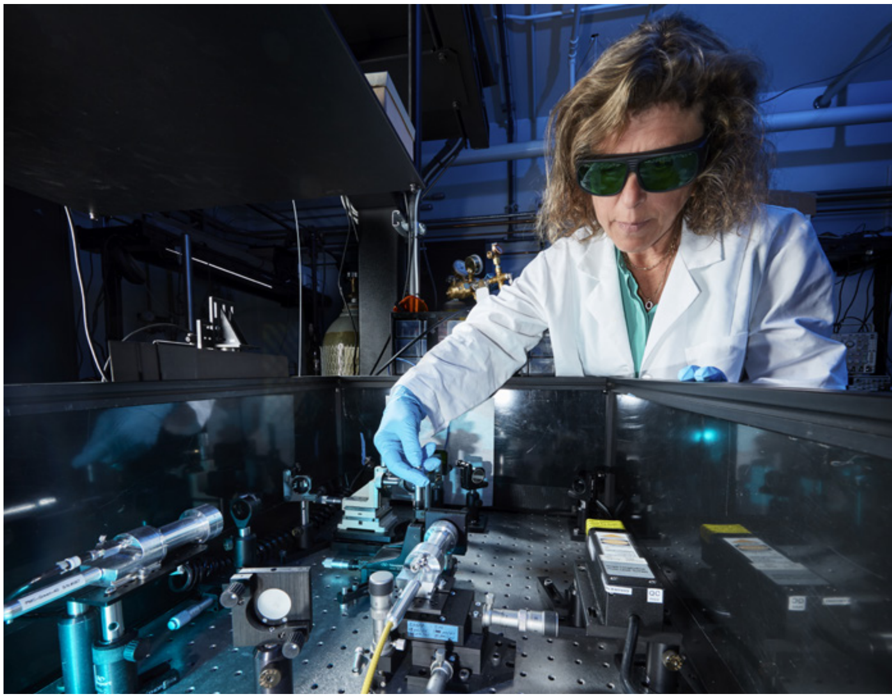


Injecting hydrogen into Earth's subsurface requires drilling a wellbore. Many reservoirs contain existing well infrastructure, but the full impact of hydrogen on the integrity of construction materials such as steel, elastomers, and cement still needs to be determined.

caprock, the geologic layer that overlays reservoirs, to maintain a seal on hydrogen. Diatomic hydrogen is the smallest molecule in existence, capable of diffusing through materials that would contain any other gaseous substance; moreover, it is highly combustible. Even if a site's caprock proves impermeable, the injected hydrogen (usually mixed with natural gas and cushion gas) could meet water, brine, or other deposits, spurring a host of geochemical reactions whose implications are not fully understood.

"UHS is a bit like the Wild West at the moment, and we don't know which potential reactions will play an important role in determining overall viability of UHS," says staff scientist Megan Smith. "Where does the hydrogen go once we've injected it into the reservoir? Does it diffuse into fine formations, like clay-rich shales? Does it react with salt formations and corrode the steel of the well-line, causing embrittlement? How does the fluid behave when we back off of the injection pressure? So many questions need answering."

Smith's team is investigating how hydrogen-rich environments affect the integrity and compatibility of natural and artificial materials in reservoirs. Using instruments purpose-built at Livermore, her team exposes geologic samples (caprock, shale, sandstone, and salt cavern deposits) and construction materials (steel and cement) obtained from project sites to different concentrations of hydrogen and reservoir brine while replicating the elevated pressures and temperatures typical of depleted gas fields: 100–170 atmospheres and 50–80°C, respectively. Thin, coupon-shaped samples are inserted into a brine- and hydrogen-filled reaction vessel that heats and pressurizes the contents while liquid and gas samples are periodically siphoned off for analysis. Smith says, "Several reactions might occur. For instance, if water evaporates, the brine's salt content will increase. If hydrogen diffuses into the brine, we will detect specific chemical analytes released from the samples as well as concentration changes to its gas phase."



Optic engineer Tiziana Bond tests fiber-optic sensors that will detect temperature, pressure, and chemical signals to constantly monitor subsurface infrastructure.

After one month, samples are removed and examined using x-ray diffraction and electron microscopy. "Quantifying surface effects gives us insight into the permeability and microporous storage of each material," says experimental scientist Maria Gabriela Davila-Ordonez. "We can relate the ion concentrations measured in fluid samples to observed changes in porous structure and mineral formation. These measurements are key to determining which materials are ideal for UHS." The team also stresses the significance of constructing the experimental facility itself. "Typically, we would use titanium vessels, but hydrogen is a different beast, mainly because of its flammability," says Smith. Stainless steel, instead, is less reactive with hydrogen. "Putting together the necessary instrumentation required many consultations with safety engineers and countless inspections to safely work with hydrogen in the laboratory," recalls Davila-Ordonez.

From Simulation to Implementation

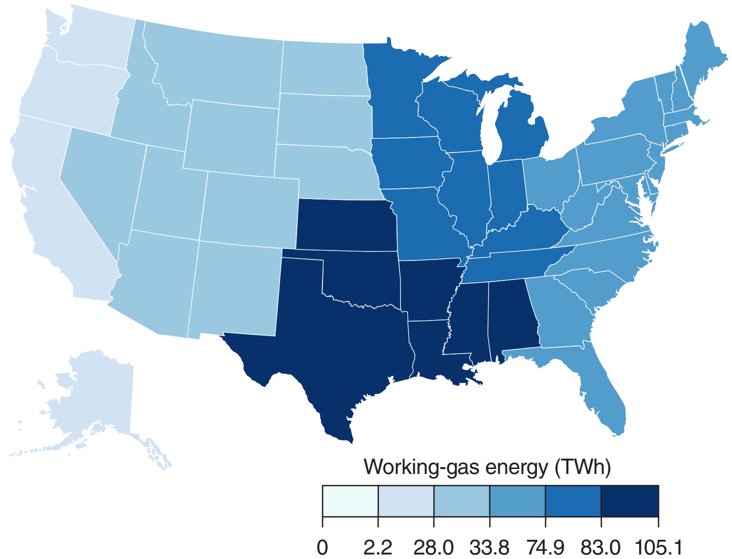
Understanding how hydrogen disperses and potentially reacts inside a reservoir is not possible without sophisticated modeling and simulation. UHS risk quantification unites benchwork and computational methods. Powering much of the digital work is GEOS, an open-source reservoir simulator developed at Livermore to understand fluid and mechanical flow of matter in Earth's subsurface. "Other commercial simulators are designed to model the movement of oil, natural gas, and carbon dioxide specifically. Hydrogen has different molecular properties and equations of state," says White. GEOS accounts for molecular differences that have pronounced macroscale effects on the movement of material mixtures. "Water, hydrogen, methane, and possibly other substances are distributed throughout the reservoir at different pressures, temperatures, and concentrations. We use compositional simulation to predict the state of each species at each timestep following hydrogen injection. Then, the 'flow step' predicts movement into neighboring cells." Crunching the numbers, researchers can identify ideal volume and timing of hydrogen injection to maximize energy storage potential at specific sites.

Beyond theoretical feasibility, SHASTA investigates practical factors for real-life implementation of UHS. For instance, ensuring the safe deployment and operation of UHS sites will demand reliable monitoring tools. Optic engineer Tiziana Bond is developing distributed fiber-optic sensors that function as the infrastructure's nervous system, detecting temperature, pressure, and chemical signals. Separated by kilometers of earth, operators must be able to detect transmission of a minuscule, transparent, odorless gas whose dispersal could cause energy resource loss and corrosion of the wellbore. "When used with imprinted gratings, fiber-optic sensors continuously emit and back-reflect specific wavelengths of light. If there were a fracture, then those vibrations will shift the associated wavelengths," says Bond. Knowing the length of the optical fiber and a signal's time of flight pinpoints anomalies in space, giving enhanced monitoring capabilities to well-drilling projects for carbon capture and sequestration.

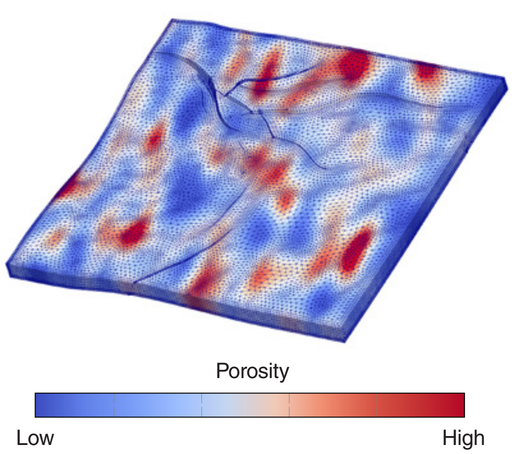
Fibers can also be used to perform chemical fingerprinting. Percolating through hollow fibers, different molecules produce unique Raman signals when intercepted by light, allowing differentiation between hydrogen, methane, and other gases. However, challenges remain. "We need to develop armor for the hollow fibers so they remain resilient during monitoring. These fibers then need to be spliced with the solid-core optical fiber." Cost is another factor, according to Bond. Lowering fiber production cost is critical because UHS sites would need kilometers upon kilometers of it to thoroughly monitor the subsurface.

The need for affordable materials underscores SHASTA's final focus: practicality and cost-effectiveness of UHS. The project's technoeconomic considerations include classifying the readiness and availability of associated technologies as well as determining the scenarios under which business would be most eager to take part in UHS projects. White explains, "We need to assess the volume and location of storage potential but also the costs associated with facility construction, material transport, energy conversion, etc., to establish a business case. As we consider deploying hydrogen technology in new areas, SHASTA will show whether our expectations are in the right ballpark."

The project's technoeconomic analysis involves classifying the readiness and availability of associated technologies as well as strategizing UHS project strategies that would most interest private businesses. In fact, UHS has already demonstrated commercial viability in salt caverns. Further study is underway to expand storage locations. Researchers must account for a spectrum of approaches to harnessing hydrogen that differ in targeted sources,



If filled with hydrogen gas, existing underground resources such as depleted oil and gas reservoirs, saline aquifers, and salt caverns distributed throughout the United States could store more than 300 terawatt-hours (TWh) of energy, enough energy to light millions of homes for a year. The shades of blue represent regional energy storage capacity expressed as the working-gas energy in TWh that could be made available.



GEOS software is a versatile tool for understanding underground fluid flow and stresses on well infrastructure. Structural permeability data, depicted here, is one input factor GEOS uses to simulate hydrogen dynamics in reservoirs as in this 2.4-kilometers-square, 300-meter-deep section.

methods of production or extraction, carbon intensity, and byproducts. As improved technologies and new experimental results continue to emerge, Livermore and its research partners regularly share data, inform stakeholders of revised scientific understanding, and recommend best practices for leveraging existing infrastructure.

DOE aims to deploy pilot projects as soon as possible to evaluate injection, monitoring, and retrieval of hydrogen at scale in a hydrocarbon reservoir, but breaking ground first requires industry buy-in and approval from both regulators and the American public. "Going forward, we will articulate the safety and benefits of hydrogen technology to the public, yet we must also sincerely listen to and consider the sentiments of people who live where these projects might take place," says White. At the intersection of Livermore's climate and energy security missions, SHASTA's multifaceted approach to realizing UHS is vital to understanding the possibilities and challenges associated with clean energy transition.

— Elliot Jaffe

Key Words: corrosion; fiber optics; GEOS; hydrogen; material compatibility; renewable energy; reservoir; Subsurface Hydrogen Assessment, Storage, and Technology Acceleration project (SHASTA); technoeconomics; underground hydrogen storage (UHS); wellbore.

For further information contact Joshua White (925) 422-3939 (white230@llnl.gov).