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Ph.D. DISSERTATION DEFENSE

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Date:	Friday, March 1st, 2024
Time/Location:	1:00 pm - 2:30 pm / https://stevens.zoom.us/j/93583800028
Title:	Investigation of Underground Hydrogen Storage using Multiscale Simulation and Machine Learning
Chairperson:	Dr. Cheng Chen, Department of Civil, Environmental and Ocean Engineering, School of Engineering and Science
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ABSTRACT

The urgent need for sustainable energy solutions against global warming has highlighted hydrogen's potential as a clean, efficient fuel. Despite its promise, the challenge of storing hydrogen on a large scale persists. Surface storage methods face limitations in capacity and practicality, thereby making underground hydrogen storage (UHS) an attractive alternative. UHS emerges as a scalable, cost-effective solution for hydrogen's long-term storage, which is crucial for achieving global-scale net-zero carbon emissions. This research explores the complex dynamics of UHS across multiple spatial scales — from the microscopic intricacies of pore-scale flows to the broader challenges of reservoir-scale storage — by utilizing a combination of numerical simulation and machine learning technologies.

By establishing a pore network model (PNM) and integrating experimental contact angle measurements, this study highlights the feasibility of using depleted gas reservoirs for UHS. Furthermore, the dissertation introduces innovative machine learning approaches, including the least square method and support vector machine, to predict hydrogen residual rates in different types of rocks. These models demonstrate remarkable alignment with PNM outcomes, thereby underscoring the potential of machine learning in guiding UHS site selections.

Additionally, pore-scale numerical simulations, complemented by high-resolution X-ray micro-computed tomography imaging and lattice Boltzmann method simulations, shed light on the role of rock surface wettability in hydrogen-brine transport in porous media. The novel fusion of Convolutional Neural Networks (CNNs) and Graph Neural Networks further advances permeability predictions, offering a memory-efficient methodology that surpasses traditional CNNs by capturing the essential connectivity and structural nuances of porous media. Building on this foundation, the dissertation extends into the reservoir scale, focusing on UHS in saline aquifers. Simulation results reveal that the choice of cushion gas significantly influences hydrogen storage dynamics, with CO_2 enhancing hydrogen solubility and reducing retrievability due to density-driven convection, which is a contrast to the behavior observed with CH_4 and N_2.

Ultimately, this dissertation not only enriches the understanding of hydrogen transport in subsurface environments but also pioneers the application of machine learning in enhancing the predictability and

efficiency of UHS. The findings and methodologies developed herein pave the way for more informed decision-making in practical UHS projects, marking a significant contribution to the field of subsurface fluid flow research.