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## Simulations of Hydrogen Storage in Sedimentary Geologic Formations

M. Delshad<sup>1</sup>, M. Mehrabi<sup>1</sup>, R. Ganjdanesh<sup>1</sup>, P. Eichhubl<sup>2</sup>, Y. Umurzakov<sup>1</sup>, and K. Sepehrnoori<sup>1</sup>

<sup>1</sup>Hildebrand Department of Petroleum and Geosystems Engineering,  
University of Texas at Austin, Austin, Texas 78712

<sup>2</sup>Bureau of Economic Geology, Jackson School of Geosciences,  
University of Texas at Austin, Austin, Texas 78758

### ABSTRACT

Hydrogen (H<sub>2</sub>) has been an attractive energy carrier and its appeal is not in just powering cars but its true potential is in decarbonizing industries such as heating of buildings and transportation fuel for trains, buses, and heavy trucks. Industry is already making tremendous progress in cutting costs and improving efficiency of hydrogen infrastructure. Currently, heating is primarily provided by using natural gas and transportation by gasoline, which have a large carbon footprint. Hydrogen has a similarly high energy density but there are technical challenges preventing its large-scale use as an energy carrier. Among these include the difficulty of developing large and reliable storage capacities.

Underground geologic storage of hydrogen could offer substantial storage capacity at low cost as well as buffer capacity to meet changing seasonal demands or possible disruptions in supply. There are several options for large-scale hydrogen underground storage: caverns, salt domes, aquifers, and depleted oil/gas fields where large quantities of gaseous hydrogen can be safely and cost effectively stored. Underground geologic storage must have adequate capacity, ability to inject/extract high volumes, and a reliable caprock. A thorough study is essential for a large number of site surveys to locate and fully characterize the subsurface geological storage sites both onshore and offshore (i.e., green hydrogen coupled with wind farms).

We have carefully evaluated existing non-isothermal compositional gas reservoir simulator(s) and their suitability for hydrogen storage and withdrawal from aquifers or depleted oil/gas reservoirs. We have successfully

calibrated the gas equation of state model against published laboratory measurements of H<sub>2</sub> density and viscosity as a function of pressure and temperature. Our numerical simulations of H<sub>2</sub> in aquifer and oil reservoirs indicated the critical need to contain the stored volume (working gas) due to H<sub>2</sub> high mobility (low density and viscosity). The latter objective can be achieved with an integrated approach of site selection and its geological features (i.e., faults/natural fractures, caprock properties), well locations, and the need for pump wells to maximize the gas capacity and displacing the in-situ fluids.

## INTRODUCTION

Hydrogen is the most plentiful element in the universe, but it must be separated from some other substance such as water or fossil fuels. For example, industries like oil refining use large quantities of hydrogen that is mostly made by separating hydrogen from natural gas. Some of its potential usages are in powering long-haul trucks, trains, and air travel. The National Aeronautics and Space Administration (NASA) began using liquid hydrogen in the 1950s as a rocket fuel and NASA was one of the first to use hydrogen fuel cells to power the electrical systems on spacecraft. Some energy companies are also looking into blending hydrogen with natural gas for home heating and cooking. Industry is already making "tremendous progress" in cutting costs and improving efficiency of hydrogen infrastructure, according to Wayne Leighty, hydrogen business development manager for Royal Dutch Shell in North America.

Natural gas reforming is an advanced and mature hydrogen production process that builds upon the existing natural gas infrastructure. Today 95% of the hydrogen produced in the United States is made by natural gas reforming in large central plants (i.e., blue hydrogen). This is an important pathway for near-term hydrogen production.

Combining these processes with carbon capture and storage will reduce the carbon dioxide emissions. Essential for successful implementation of the hydrogen economy is field-proven technologies to store large quantities of hydrogen underground in solution-mined salt domes, saline aquifers, excavated rock caverns, depleted oil/gas reservoirs, or mines to act as a grid energy storage.

There are several options for large-scale seasonal hydrogen underground storage namely manmade caverns, salt domes, aquifers, and depleted oil/gas fields. Large quantities of gaseous hydrogen have been stored in salt caverns for many years. The Chevron Phillips Clemens Terminal in Texas has stored hydrogen since the 1980s in a solution-mined salt cavern. The cavern is about 2800 ft underground, in the shape of a cylinder having a diameter of 160 ft, and can hold 2520 metric tons storage capacity. RAG Austria AG finished a hydrogen storage project in a depleted oil and gas field in Austria in 2017. Their research included developing and testing technology for storing wind and solar energy by converting electrical energy into hydrogen, so that the existing natural gas field could be used as seasonal storage for surplus energy from renewable energy sources.

## METHODS

In this research, we used an existing non-isothermal compositional gas reservoir simulator for modeling hydrogen storage and withdrawal from depleted oil/gas reservoirs and/or aquifers based on the seasonal energy need. The process requires laboratory data to obtain phase behavior and fluid property model parameters for hydrogen/oil/water system and density, viscosity, and solubilities in brine and oil. We simulated hydrogen injection and withdrawal in several potential storage sites having different geologic characteristics. We developed strategies for optimum energy storage and withdrawal and investigated the impact of up-coning of water/gas and water displacement.

**RESULTS**

**Hydrogen-Water Phase Behavior and Properties**

It is important to understand the phase behavior and properties of hydrogen in comparison with CO<sub>2</sub> and methane as a function of pressure at a given reservoir temperature. The density of H<sub>2</sub> was tuned at reservoir conditions using the Peng-Robinson equation-of-state and volume shift parameters. **Figure 1** shows that the tuned model can match the experimental data (Lemmon et al, 2008; NIST, 2021; Muzny et al., 2013; Yusibani et al., 2011) of density at subsurface temperature and a wide range of pressure. The viscosity of H<sub>2</sub> was tuned using the Lohrenz-Bray-Clark (LBC) model (Lohrenz et al., 1964). **Figure 2** shows that the tuned model matches the experimental data with high accuracy. **Figure 3** compares the density of H<sub>2</sub>, CH<sub>4</sub>, and CO<sub>2</sub>. At similar conditions, the density of H<sub>2</sub> is about 10 times less than the density of CH<sub>4</sub> and about 30 times less than the density of CO<sub>2</sub>. **Figure 4** shows that the viscosity of H<sub>2</sub> at reservoir conditions can be 2-3 times less than the viscosity of CH<sub>4</sub> and 5-10 times less than that of CO<sub>2</sub>.

**Simulation Study of Different Storage Sites**

We selected one saline aquifer that was used as a CO<sub>2</sub> storage demonstration pilot and one natural gas storage site to study as hypothetical storage candidates for H<sub>2</sub>.

**Case 1: Saline Aquifer Frio Site, Gulf Coast**

The Frio is part of a thick extensive sandstone with numerous shale seals and faults that underlies industrial sources and power plants along the Gulf Coast of the United States. The Frio has been used as a demonstration project for CO<sub>2</sub> storage in a saline aquifer, in which about 1600 metric tons of CO<sub>2</sub> was injected in 10 days (Hovorka, et al., 2006). The initial pressure is 150 bars, reservoir temperature is 55°C, and water salinity is 100,000 ppm. Many research groups have modeled and history matched the results of the Frio CO<sub>2</sub> demonstration. **Figure 5** gives the schematic of the formation, where CO<sub>2</sub> was injected, porosity distribution, and several faults.

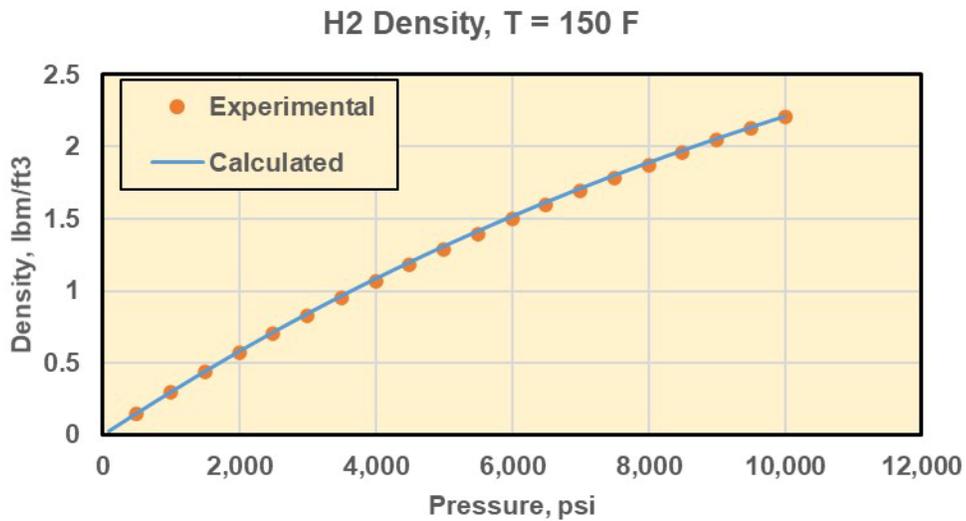


Figure 1. Calculated H<sub>2</sub> density vs. pressure at 150°F.

### H2 Viscosity, T = 150 F

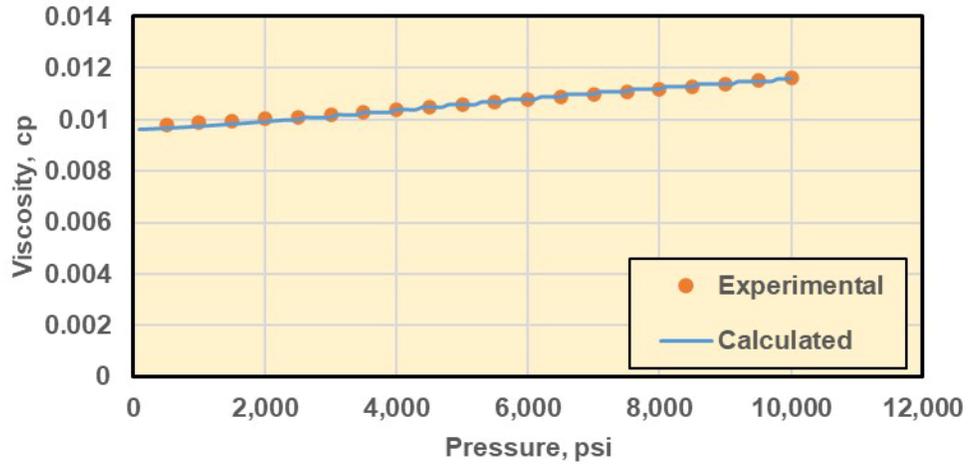


Figure 2. Calculated H<sub>2</sub> viscosity vs. pressure at 150°F.

### H2 vs CH4 vs CO2 Density

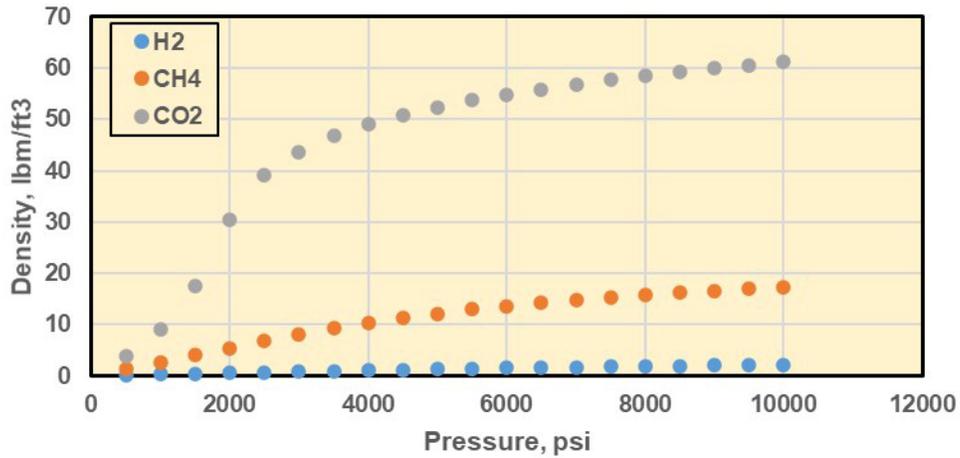


Figure 3. Density comparison for H<sub>2</sub> against CO<sub>2</sub> and methane vs. pressure at 150°F.

We used the history matched Frio numerical model for H<sub>2</sub> storage and observed very different results of the plume extension and distribution of these gases. H<sub>2</sub> occupied more volume with higher pressure due to its higher mobility and significantly lower viscosity and density compared to CO<sub>2</sub>. [Figure 6](#) compares the plume for both gases. Of course, for H<sub>2</sub>, we store, redistribute, and produce back in multiple cycles whereas CO<sub>2</sub> storage involves only injection and redistribution.

## H2 vs CH4 vs CO2 Viscosity

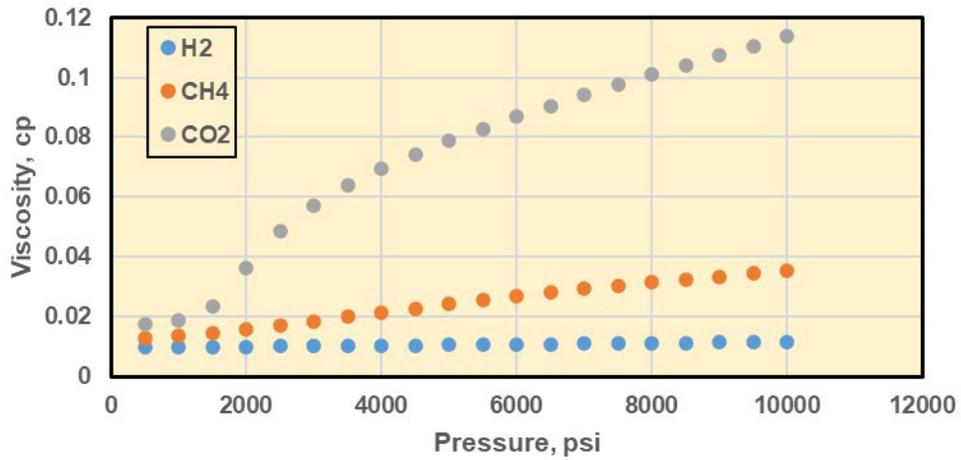


Figure 4. Viscosity comparison for H<sub>2</sub> against CO<sub>2</sub> and methane vs. pressure at 150°F.

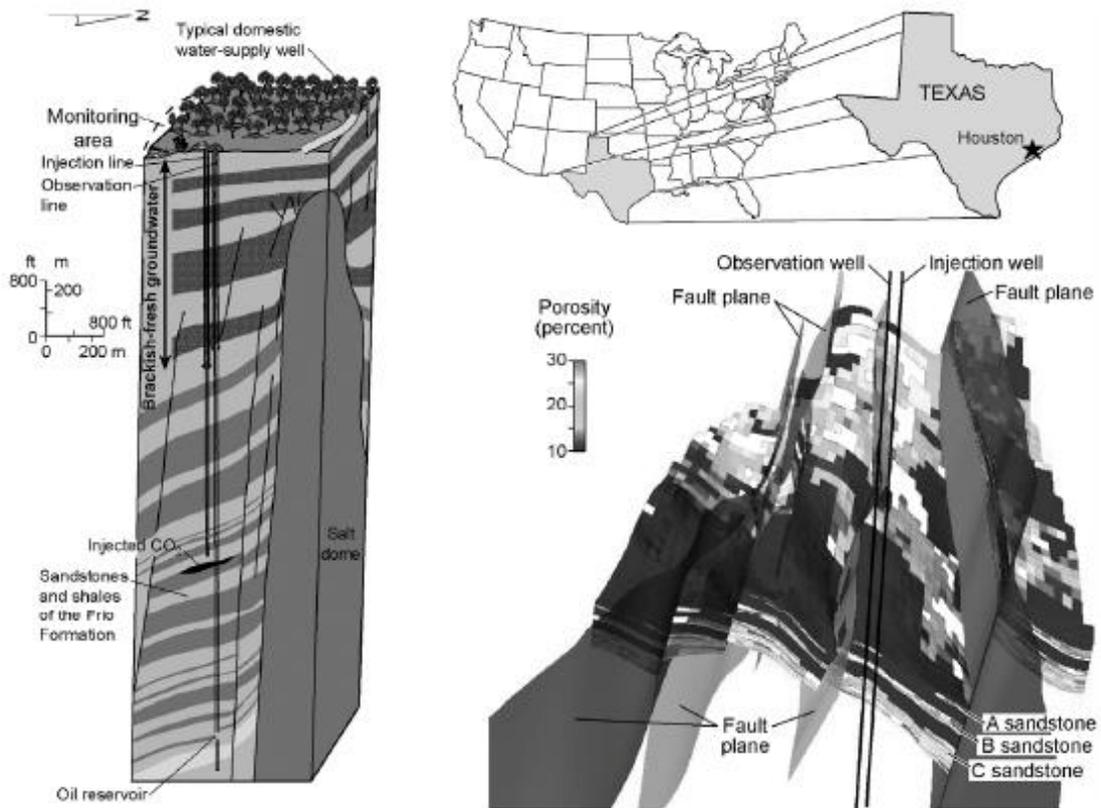


Figure 5. Frio CO<sub>2</sub> demonstration site showing geologic context near South Liberty Salt Dome and detail of injection well location within a gridded reservoir model made using seismic data of the fault block (Hovorka et al., 2006).

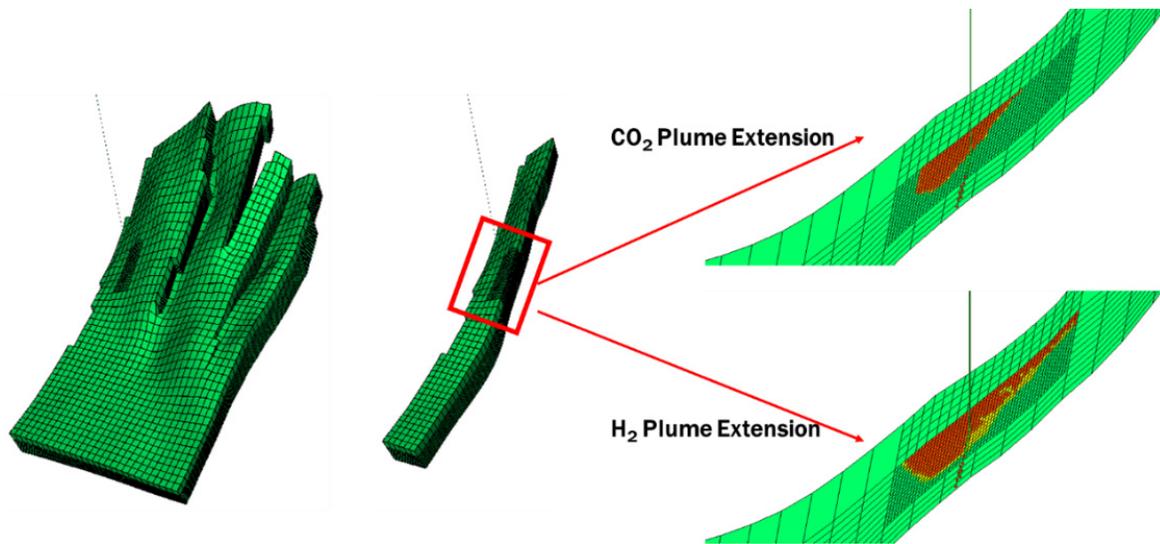


Figure 6. Numerical model and comparison of CO<sub>2</sub> plume (upper right-hand side image highlighted in red) and H<sub>2</sub> plume (lower right-hand side image with H<sub>2</sub> plume highlighted in red) in Frio model.

### Case 2: Natural Gas Storage, Colorado

This test case was based on an actual natural gas storage site in Colorado. The oil reservoir was waterflooded for many years until 2011. The gas-oil ratio is 457 standard cubic ft/bbl, the bubble point pressure is 1240 psig, and the oil American Petroleum Institute (API) gravity is 37 deg. The reservoir consisted of a channel sand having 400 md permeability and non-channel sand having 10 md permeability (Fig. 7). There were several injection wells in the dome of the channel sand that were also used to withdraw gas. In order to increase the working gas volume, additional wells (pump wells) were utilized during the injection cycle to produce water and oil so as to provide more storage capacity while natural gas was being injected.

We performed compositional reservoir simulations comparing the storage performance of H<sub>2</sub> and natural gas. The results indicated about 10% less volume of H<sub>2</sub> were stored compared to the natural gas, 32% less working gas capacity, and 5% less oil production. H<sub>2</sub> was more buoyant and migrated more rapidly towards the top of the dome; nearly 3% higher saturation in the top layer due to its lower density. Figures 8-9 compare the saturation distributions where H<sub>2</sub> clearly has a larger swept volume, is less confined, and spreads through the channel sand.

Additional simulations were performed to assess the impact of the number of injection wells, well orientation (horizontal wells), perforations in different layers, relative permeability, capillary pressure, the presence of the oil phase, the number and operation of pump wells, and the number of injection/withdrawal cycles (Fig. 10).

### SUMMARY AND CONCLUSIONS

Despite vast experience of storing CO<sub>2</sub> and natural gas in different geological settings of saline aquifers and depleted oil/gas reservoirs, H<sub>2</sub> storage has its own challenges and more Re-

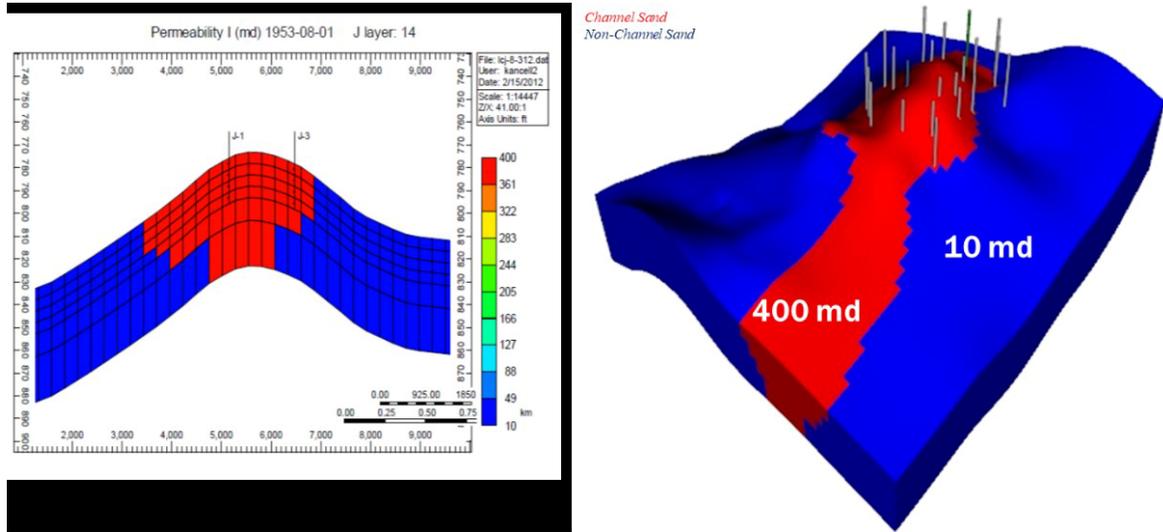


Figure 7. Reservoir model for natural gas storage site. The permeability contrast of channel (red color) and non-channel (blue color) sands are highlighted in both vertical (left image) and areal cross sections (right image).

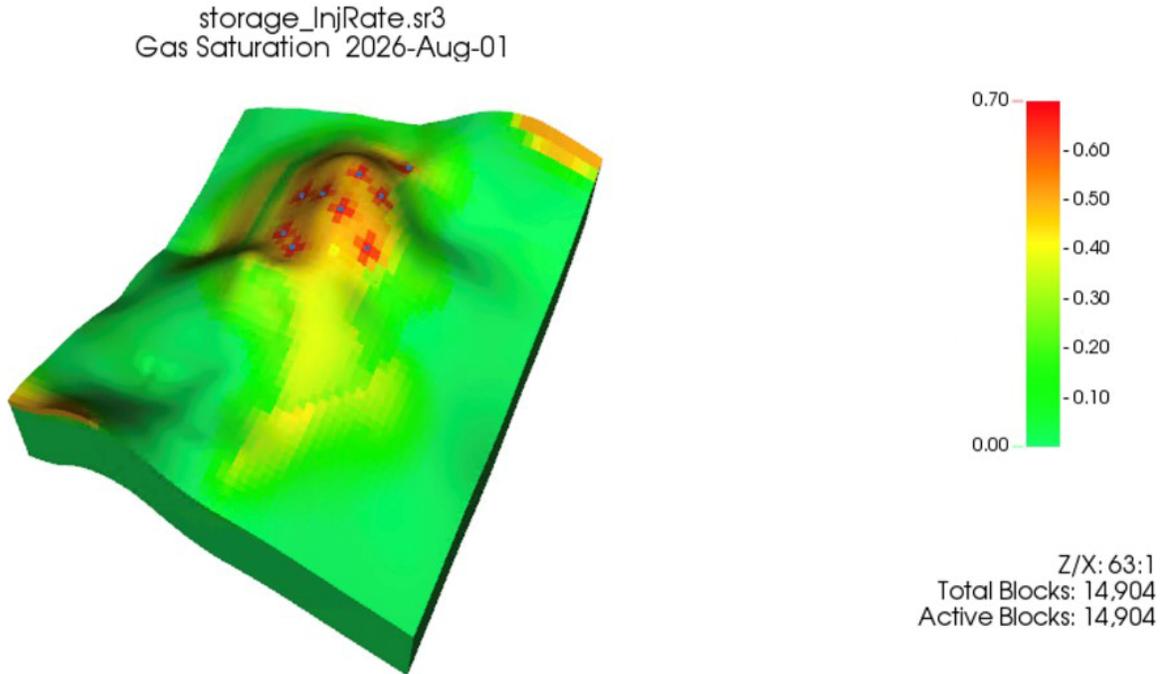


Figure 8. Natural gas saturation distribution indicating higher gas saturation in the dome of the channel sand.

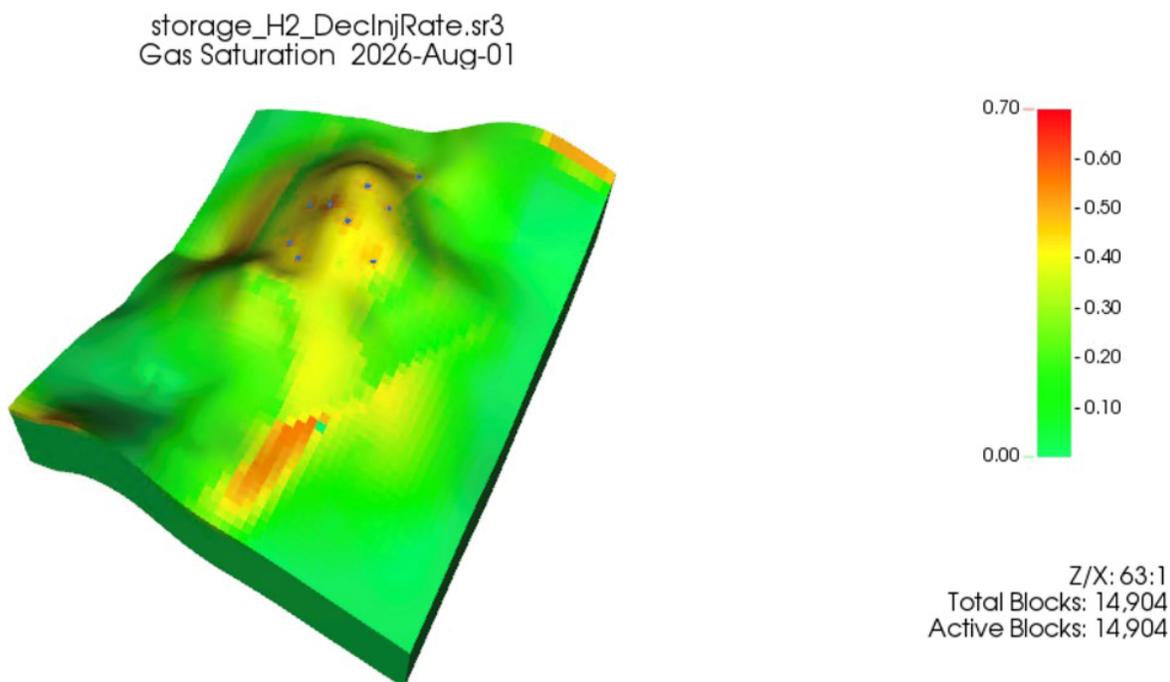


Figure 9. H<sub>2</sub> saturation distribution indicating the hydrogen movement down dip in the high permeability channel sand.

search is needed to select, design, and execute efficient and safe storage projects. Some of these challenges and future research studies are:

- Impact of H<sub>2</sub> properties on swept volume and its containment in contrast to carbon dioxide and methane storage,
- Suitability of saline aquifers compared to depleted oil or gas reservoirs considering storage integrity, mixed gases, and potential impact of H<sub>2</sub> on rock properties,
- Managing large variations in volumes/rates to load and unload,
- Impact of H<sub>2</sub> purity on fluid separation and transport, and
- Assessment of leakage and mitigation strategies.

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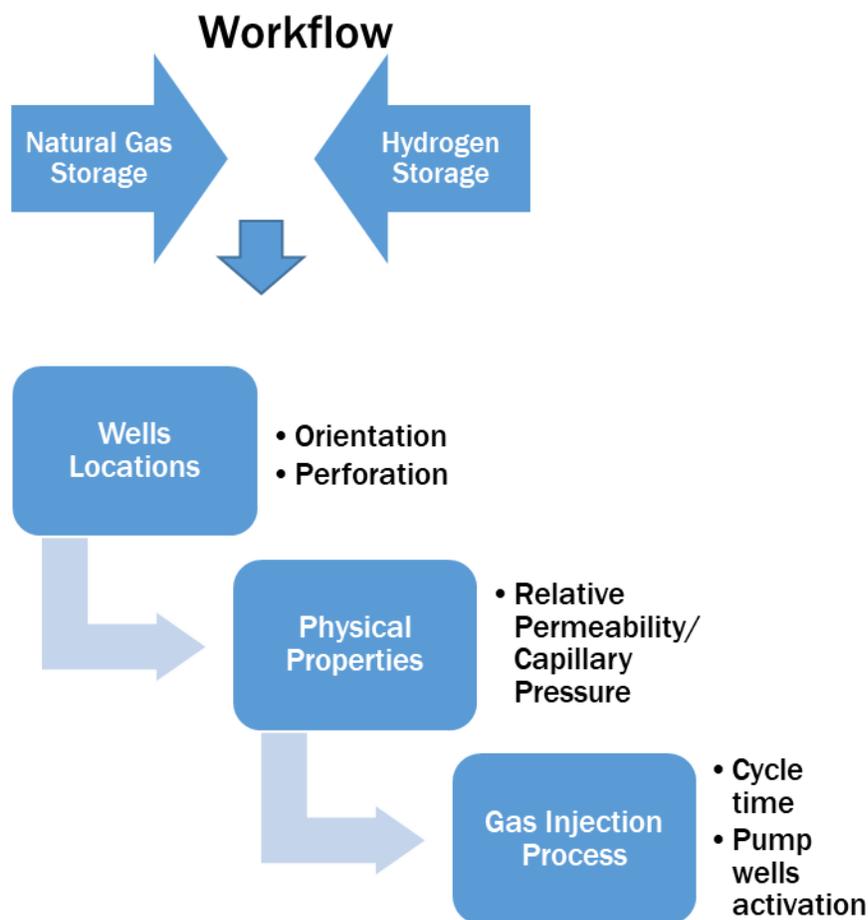


Figure 10. Diagram for H<sub>2</sub> storage optimization workflow.

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## NOTES

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