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Hydrogen flow and trapping in sandstone rocks: Comparing pore-scale experiments with pore network modelling

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Summary

Understanding pore-scale hydrogen displacement and trapping is crucial for developing subsurface hydrogen storage facilities. While pore-scale flow visualization experiments provide critical insights, they are complex and resource-intensive. Quasi-static pore-network models (PNMs) offer a faster alternative for simulating multiphase flow. This study uses a widely employed PNM to simulate hydrogen flow in sandstones, comparing results with pore-scale flow visualization experiments at reservoir conditions.

Two sandstone samples were used: homogeneous Bentheimer and heterogeneous Clashach. Pore networks were extracted comprising pores and throats, and hydrogen-water flow was simulated, modelling drainage and imbibition processes. Results were analysed for fluid saturations and pore occupancies.

For the homogeneous rock, the PNM matches experimental results for both drainage and imbibition, enabling simulations of different wettability conditions and multiple injection and production cycles. For the heterogeneous rock, the PNM reasonably predicts the hydrogen flow path during drainage but fails to accurately predict imbibition. This discrepancy highlights the limitations of PNMs in predicting pore-scale flow in complex rocks.

In conclusion, while PNMs offer a computationally efficient means to simulate hydrogen flow, they cannot currently replace experimental observations for complex rocks. Further validation against experimental findings is necessary to refine these models and expand their applicability for underground hydrogen storage.

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Introduction

Subsurface porous rocks can store substantial volumes of hydrogen (H_2) crucial for a H_2 economy transition [Miocic et al., 2023]. Understanding the pore-scale displacement and trapping mechanisms for H_2 in these rocks is vital for developing subsurface H_2 storage facilities [Tarkowski and Uliasz-Misiak, 2022; Zivar et al., 2021]. Pore-scale flow visualization experiments are essential for comprehending these mechanisms but are intricate and resource-intensive under subsurface conditions.

Quasi-static pore-network models (PNMs) offer a faster alternative for understanding multiphase flow in porous media. These models represent pore spaces as networks of pores and throats with idealized geometries, simulating fluid invasion based on capillary pressure [Bultreys et al., 2018]. PNMs have been extensively used for oil-water systems to estimate macroscopic properties [Bultreys et al., 2020]; however, their use for H_2-water systems remains limited.

In this work, we use a widely employed PNM [Bultreys et al., 2018; Raeini et al., 2017; Valvatne and Blunt, 2004] to simulate H_2 flow in two distinct networks, one from a homogeneous rock sample and another from a heterogeneous layered rock sample. The simulated results are compared with recent pore-scale 3D visualization experiments on both rocks [Jangda et al., 2023, 2024]. The PNM also allows us to evaluate the effects of varying contact angle on fluid flow behavior under different wettability conditions and simulates multiple flow cycles to mimic field H_2 storage and withdrawal processes.

Materials and methods

Two different sandstone rock samples were used in this work. A homogeneous Bentheimer sandstone, and a layered Clashach sandstone. 6 mm diameter core samples were prepared and used for pore-scale H_2 flow visualization experiments performed at reservoir conditions of 50°C and 100 bar in a flow system inside a micro-CT X-ray machine. Hydrogen was injected into the initially water saturated cores (drainage) and then water was injected to produce back H_2 (imbibition). The cores were scanned after each injection step to capture fluid distributions, which were analysed to visualize and quantify fluid saturations and pore occupancies. Our previous works [Jangda et al., 2023, 2024] provide detailed insights into these experiments, highlighting the impact of pore-scale displacement mechanisms, such as potential H_2 dissolution in water and pore-scale heterogeneity on H_2 flow and trapping in the rock pores.

To evaluate a PNM against our experimental results, multiple flow simulations were performed. Pore networks were extracted using an open-source code [Bultreys et al., 2018, 2020; Raeini et al., 2017], and H_2-water flow was simulated using an open-source pore-flow simulation model [Bultreys et al., 2018; Valvatne and Blunt, 2004]. Initially, all elements in the network model contain water. For drainage, throats along the inlet face are assumed to be connected to a H_2 reservoir, with H_2 pressure increased while water pressure remains constant. This raises the capillary pressure, filling pores and throats in order of increasing capillary entry pressure, until the predefined H_2 saturation, matching the experimental observations is reached. The model incorporates wetting layers, positioning H_2 in the centre of the network elements (pores and throats), and water remains in the corners, ensuring global connectivity and minimal water trapping during drainage.

For imbibition, water is introduced by increasing the water phase pressure while keeping the H_2 phase pressure constant through the outlet reservoir, leading to a decreased capillary pressure. Displacement events are organized based on their entry capillary pressure, with the highest capillary pressure event executed first. During imbibition, snap-off events reduce H_2 connectivity, leading to H_2 entrapment in the pore space.

Results

The flow simulation model generated output files at each step, detailing which pores and throats were filled with H_2 or brine. These were used to create images for visualizing fluid phases and analysing H_2 saturation and pore occupancy.

For the homogeneous rock sample, the H_2 saturation profiles show reasonable agreement between the experimental and simulation results after both drainage and imbibition as shown in Figure 1A and B.

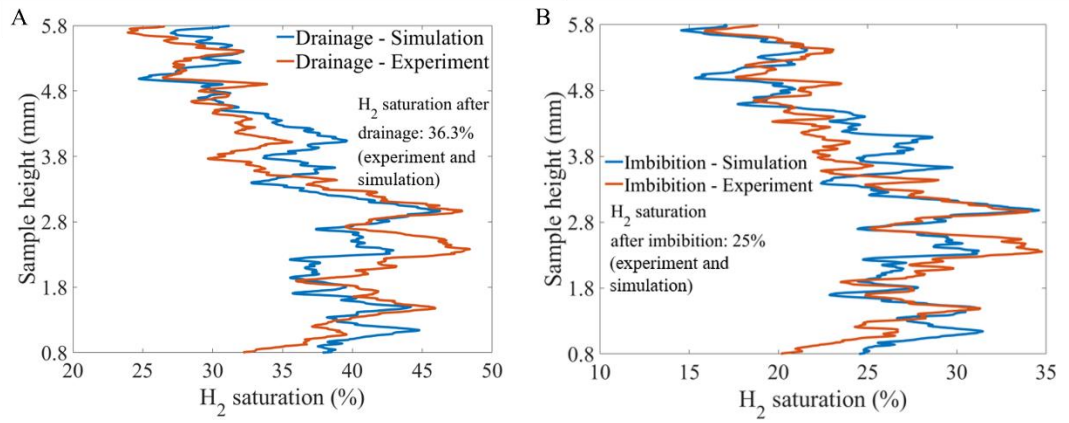

Figure 1 *Hydrogen saturation profile plotted along the height of the homogeneous rock sample (simulation and experiment), (A) after drainage and (B) after imbibition.*

H_2 remained as a single connected phase after drainage and as multiple disconnected trapped ganglia after imbibition, though there was a visual mismatch in fluid distribution, particularly in ganglia distributions (Figure 2A-D). This discrepancy is attributed to multiple network elements having similar statistical properties, leading to divergent paths for fluid invasion. This means that although statistically comparable, the simulation model does not precisely match the experimental results concerning fluid distributions on a pore-by-pore basis.

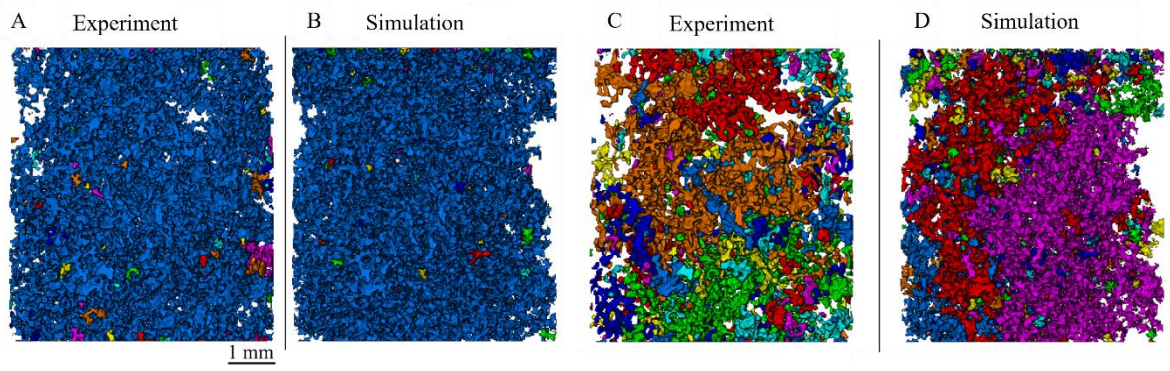

Figure 2 *Hydrogen phase visualised in the pore space of the homogeneous rock sample, (A) after drainage – experiment, (B) after drainage – simulation, (C) after imbibition - experiment and (D) after imbibition - simulation.*

The reasonable agreement of the PNM with the homogeneous rock experiment allows us to simulate different wettability conditions by adjusting the contact angle. This sensitivity study predicts H_2 flow behavior under various wettability scenarios. Additionally, the PNM can simulate multiple injection and production cycles, mimicking the hydrogen storage and production life cycle in an underground storage system. While conducting these steps experimentally is challenging and resource-intensive, using the PNM helps us understand changes in storage and recovery over multiple flow cycles.

Next the simulation model was used to predict fluid displacements within the more complex pore network extracted from the heterogeneous rock sample. This rock sample features a thin low-

permeability layer sandwiched between two thicker layers with higher permeability. The middle low-permeability layer contains a pathway of larger pores, facilitating H_2 connectivity between the top and bottom layers during drainage in the experiment (Figure 3A). This slight structural heterogeneity had a significant effect on fluid distributions during the experiment.

The model accurately predicted H_2 flow through the preferential pathway in the middle layer during drainage (Figure 3B) but failed to match experimental results during imbibition (Figure 3C and D). While the model does indicate snap-off events in the middle layer, it fails to align reasonably with the experimentally observed results.

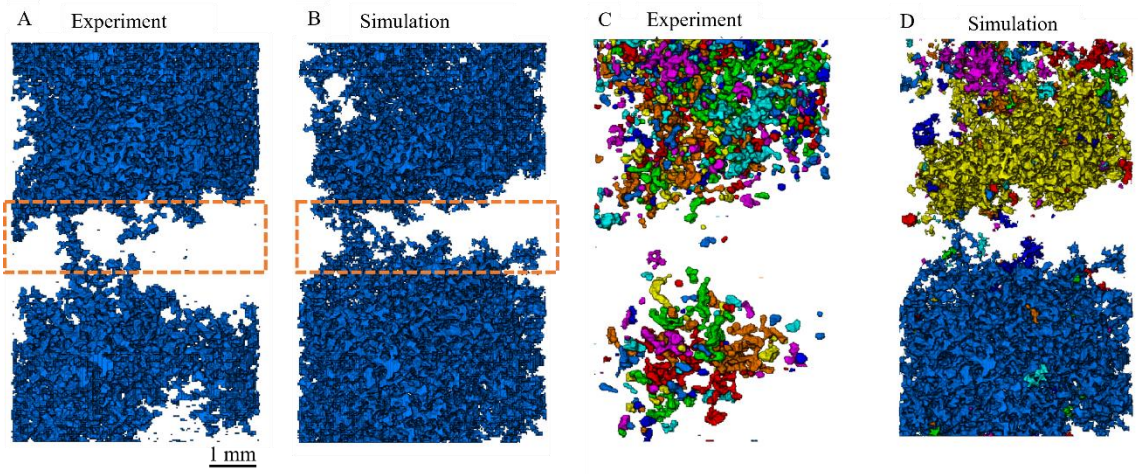

Figure 3 *Hydrogen phase visualised in the pore space of the heterogeneous rock sample, (A) after drainage – experiment, (B) after drainage – simulation, (C) after imbibition - experiment and (D) after imbibition - simulation. The middle low permeability layer is highlighted with orange dashed lines in (A) and (B).*

The H_2 saturation profiles predicted by the model differ considerably from the experimentally observed results particularly for imbibition (Figure 4A and B).

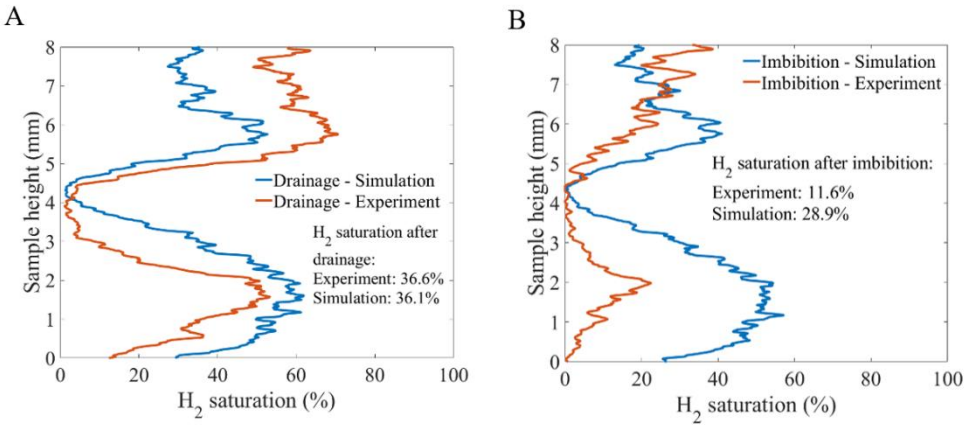

Figure 4 *Hydrogen saturation profile plotted along the height of the heterogeneous rock sample (simulation and experiment), (A) after drainage and (B) after imbibition.*

The discrepancies in simulation results highlight the limitations of PNMs in accurately predicting pore-scale flow properties during imbibition [Bultreys et al., 2020; Ellman et al., 2024], especially in heterogeneous rocks. The model not only has to be statistically accurate for the entire network, but also requires to precisely depict flow and trapping within the same network elements controlling fluid displacement during the experiment. Moreover, the existing inconsistency between experimental and simulated results after drainage for the heterogeneous rock, makes the accurate prediction of imbibition with the simulation model even more challenging.

Conclusion

Comparative analysis indicates good agreement between PNM simulations and experimental results for drainage and imbibition in the homogeneous case, and reasonable agreement for drainage in the heterogeneous case. However, it is apparent that while PNMs offer a simplified and computationally efficient means to simulate H_2 flow and displacement in porous media, they cannot presently supplant experimental observations, particularly for complex rocks. Further validation against experimental findings is necessary to refine these models, enabling them to accurately predict macroscopic properties such as relative permeability and capillary pressure for H_2-water systems, thereby expanding their applicability.

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