

## Pore-Scale Numerical Simulation of Hydrogen Gas Capillary Trapping in Natural Sandstone under In-Situ Wettability Conditions (Postprint)

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### Abstract

A deep understanding of the hydrogen capillary trapping mechanism under in-situ wettability conditions of natural rocks is crucial for improving hydrogen recovery during hydrogen storage in aquifers. In this study, sandstone hydrogen-water displacement experiments were conducted under reservoir in-situ temperature and pressure conditions, and hydrogen-water distribution images inside the sandstone during the displacement process were obtained through micro-CT scanning. Based on the obtained hydrogen-water distribution images, the in-situ contact angle of the hydrogen-water-sandstone system was determined, and a microscale pore model of the sandstone was reconstructed. An in-situ wettability modeling method for pore-scale hydrogen-water two-phase flow was proposed based on the determined in-situ contact angle and the Volume of Fluid (VOF) method, and its effectiveness was validated through experimental results. The hydrogen capillary trapping phenomenon during spontaneous and forced imbibition in sandstone under in-situ wettability conditions was simulated and studied, and the influence of water injection rate and gas-water interfacial tension on hydrogen recovery was analyzed and discussed. The results show that: (1) The hydrogen-water-sandstone multiphase system exhibits heterogeneous water-wet characteristics, and the in-situ wettability modeling method proposed in this paper can effectively predict the hydrogen-water two-phase flow process in natural rocks; (2) The growth and accumulation of water films in throats with large pore-throat ratios is the main cause of hydrogen snap-off and capillary trapping; (3) During the water-drive-gas process, hydrogen residual saturation and gas-water interfacial area decrease with increasing water injection rate; (4) The slight reduction in gas-water interfacial tension caused by methane buffer gas contributes negligibly to improving hydrogen recovery in aquifers.

## Full Text

### Pore-scale numerical investigation on the capillary trapping of hydrogen in natural sandstone under in-situ wettability conditions

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## Abstract

A comprehensive understanding of hydrogen capillary trapping mechanisms in natural rocks under in-situ wettability conditions is essential for enhancing hydrogen recovery efficiency in underground aquifer storage. This study conducted hydrogen-displacing-water experiments in sandstone under reservoir temperature and pressure conditions, utilizing micro-CT scanning to capture the internal hydrogen-water distribution during the displacement process. Based on these images, we determined the in-situ contact angles of the hydrogen-water-sandstone system and reconstructed a microscale pore model of the sandstone.

We subsequently developed a pore-scale modeling approach for hydrogen-water two-phase flow under in-situ wettability conditions by integrating the obtained contact angles with the Volume of Fluid (VOF) method. The validity of this methodology was confirmed through comparison with experimental results. Using this approach, we numerically investigated hydrogen capillary trapping phenomena during both spontaneous and forced imbibition in sandstone under in-situ wettability conditions, and systematically analyzed the influence of water injection rate and gas-water interfacial tension on hydrogen recovery.

The results reveal four key findings: (1) The hydrogen-water-sandstone multiphase system exhibits heterogeneous water-wet characteristics, and the proposed in-situ wettability modeling approach can effectively predict hydrogen-water two-phase flow processes in natural rocks. (2) The growth and accumulation of water films in throats with large pore-throat ratios constitute the primary mechanism responsible for hydrogen snap-off and subsequent capillary trapping. (3) During water-displacing-gas processes, both residual hydrogen saturation and gas-water interfacial area decrease as the water injection rate increases. (4) The slight reduction in gas-water interfacial tension caused by methane buffer gas contributes negligibly to improving hydrogen recovery in aquifer storage systems.

**Keywords:** Capillary trapping; In-situ wettability; Underground hydrogen storage; Hydrogen-water two-phase flow; Pore-scale modeling; Imbibition

*Note: Figure translations are in progress. See original paper for figures.*

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