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Volume of Fluid based study of the three phase dynamic contact line on rough surfaces relevant for Underground Hydrogen Storage

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Large-scale (TWh) renewable energy storage is crucial to achieve a net-zero green world. To accomplish this, renewable energy can be converted into hydrogen (H_2) and stored in large-scale volumes in giant subsurface geological reservoirs. The feasibility of underground hydrogen storage in porous reservoirs highly depends on the flow and transport behaviour of hydrogen during subsequent injection and withdrawal cycles in the reservoir, which is governed by complex pore-scale processes [1-3].

Recently, several experimental studies [4-8] have taken place, which allow for the characterization of hydrogen transport properties in the subsurface. However, some discrepancies were found in contact angle characterization results using different measurement techniques and solid surfaces. The roughness of the solid surface is a possible explanation for this [9]. To date, no study has investigated the impact of roughness on the characterization of H_2-brine flow.

To help shed new light on the characterization of this crucial property, the Basilisk flow solver is used to conduct numerical simulations by solving the 2D two-phase Navier-Stokes equation. The H_2-brine interface is captured using the Volume-of-Fluid method, and the Continuous Surface Force method is employed to compute surface tension forces. The calculation of the curvature is done using height functions. To investigate the influence of surface roughness on H_2-brine flow in sandstone channels, a hybrid Volume-of-fluid coupled embedded boundary solver is used. Within this solver, an intrinsic contact angle can be imposed on solids with diverse shapes, facilitating the replication of a rough sandstone surface. Dynamic contact line motion and apparent contact angles can be analysed.

By comprehending the influence of surface roughness on the contact line motion, we will gain insight into the reported experimental measurements and assess the appropriateness of using specific data as input for larger-scale simulations.

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