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Modelling liquid-gas interface movement under imbibition conditions considering solubility effects

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The geological storage of CO2 involves the interaction of non-equilibrated fluids (connate water and injected fluid) which then equilibrate over time. The CO2 phase diagram and solubility of CO2 in water adds significant complexity to this process. Namely, the existence of concentration gradients surrounding fluid-fluid interfaces may impact on wettability or more general on surface conditions. These pore-scale mechanisms make the prediction of fluid movements a challenging task.

Our research investigates the behaviour of the gas-liquid interface due to the variation in solubility dynamics by numerically simulating the spontaneous capillary imbibition of water into a gas-filled medium. An opensource simulation software featuring the "hybridPorousInterFoam" package is utilized, where the formation of two-phase interfaces is achieved by setting the initial fluid distribution and using the VOF (Volume of Fluid) method to calculate the liquid volume fraction in each cell, thereby accurately tracking the fluid-gas interface positions between as well as calculating the changing fractional fluid composition on either side of the moving interface. Subsequently, the simulation accurately reflects the physical behaviour at these interfaces by incorporating the effects of capillary forces and gravity.

This package allows the input of a distribution of contact angles to set the boundary conditions on the solid surface. Here we introduce additional functionality to model the concentration gradient evolution around the moving interfaces and account for the change in contact angles accordingly.

We demonstrate the capabilities of the new solver packages on a set of basic geometries, investigating the impact of solubility (e.g., due to temperature variations) on the resultant fluid configurations and displacement efficiency.

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References

Carrillo, F. J., Bourg, I. C., & Soulaine, C. (2020). Multiphase flow modeling in multiscale porous media: An open-source micro-continuum approach. Journal of Computational Physics: X, 8, 100073.

Conference Proceedings

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