THERMODYNAMIC MODELING AND NUMERICAL SIMULATION OF HYDROGEN STORAGE IN SALINE AQUIFERS

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ABSTRACT

This study focuses on modeling hydrogen (H2) storage in subsurface formations, specifically examining the equilibrium dynamics between H2 and brine and their impact on hydrogen transport properties in black-oil reservoir simulations. We begin by evaluating and refining various equations of state (EoS) for H2-water and H2-brine mixtures, including molecular-level models such as Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT), explicit Redlich-Kwong cubic EoS, and an empirical Setchenow-Henry model. These models are rigorously compared in their ability to predict mutual solubilities, validated against experimental data, demonstrating strong predictability across diverse conditions of temperature, pressure, and salinity with a modest number of adjustable parameters.

Subsequently, we apply these thermodynamic models to generate Pressure-Volume-Temperature (PVT) phase equilibrium data for incorporation into black-oil simulations, modeling H2 behavior in saline aquifers. We investigate the effects of salt concentration, H2 solubility, molecular diffusion, as well as cycling frequency, injection, and withdrawal rates on the storage and recoverability processes. Several numerical examples are presented to illustrate a range of complexities, including heterogeneous permeability, porosity variations, and diverse rock types with specific entry pressures, providing a comprehensive exploration of the factors influencing H2 storage in subsurface formations.

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