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Behavior of water in supercritical CO_2: adsorption and capillary condensation in porous media

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The chemical potential of water in supercritical CO_2 ($scCO_2$) may play an important role in water adsorption, capillary condensation, and evaporation under partially saturated conditions at geologic CO_2 storage sites, especially if initially anhydrous CO_2 is injected. Such processes may affect residual water saturations, relative permeability, shrink/swell of clays, and colloidal transport. We have developed a thermodynamic model of water or brine film thickness as a function of water relative humidity in $scCO_2$. The model is based on investigations of liquid water configuration in the vadose zone and uses the augmented Young-Laplace equation, which incorporates both adsorptive and capillary components. The adsorptive component is based on the concept of disjoining pressure, which reflects force per area normal to the solid and water/brine-$scCO_2$ interfaces. The disjoining pressure includes van der Waals, electrostatic, and structural interactions. The van der Waals term includes the effects of mutual dissolution of CO_2 and water in the two fluid phases on partial molar volumes, dielectric coefficients, and refractive indices. Our approach treats the two interfaces as asymmetric surfaces in terms of charge densities and electrostatic potentials. We use the disjoining pressure isotherm to evaluate the type of wetting (e.g., total wetting or partial wetting) for common reservoir and caprock minerals and kerogen. The capillary component incorporates water activity and is applied to simple pore geometries with slits and corners. Finally, we compare results of the model to a companion study by the coauthors on measurement of water adsorption to mineral phases using a quartz-crystal microbalance.

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