ADSORPTION OF METHANE AND CO2 IN GAS SHALES FROM EXPERIMENTS TO MOLECULAR SIMULATIONS

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One method for mitigating the impacts of anthropogenic CO_2-related climate change is the sequestration of CO_2 in depleted gas and oil reservoirs, including shale. The accurate characterization of the heterogeneous material properties of shale, including pore volume, surface area, pore size distributions and composition is needed to understand the interaction of CO_2 with shale.

This study examines two Eagle Ford shale samples, both recovered from shale that was extracted at depths of approximately 3,800 meters and having low clay content (i.e., less than 5%), similar mineral composition, but with distinct total organic content, i.e., 2% and 5%. Experimentally-validated models of kerogen were used to estimate CH_4 and CO_2 adsorption capacities. Given the presence of water in these natural systems, the role of surface chemistry on modeled kerogen pore surfaces was investigated. Several functional groups associated with surface-dissociated water were considered. Pressure conditions from 10 bar up to 50 bar were investigated along with typical outgassing temperatures used in many shale characterization and adsorption studies, i.e., 60 ℃ and 250 ℃. Both CO_2 and N_2 were used as probe gases to determine the total pore volume available for gas adsorption spanning pore diameters ranging from 0.3 nm up to 30 nm. The impacts of surface chemistry, outgassing temperature, and the inclusion of nanopores less than 1.5 nm were determined for applications of CH_4 and CO_2 storage from samples of the gas-producing region of the Eagle Ford shale.