



Contribution ID: 861

Type: Oral Presentation

Molecular Simulation of Competitive Adsorption of H₂S-Containing CO₂ and CH₄ in Organic and Inorganic Shale Nanopores

Monday, 13 May 2024 13:40 (15 minutes)

Objectives/Scope:

Geological storage of acidic gases can reduce atmospheric emissions of CO₂ and H₂S, thus serving as a critical part of low-carbon energy systems. Depleted shale gas reservoirs are good storage candidates owing to their intrinsic gas storage capacity. However, shales exhibit complex structural characteristics and abundant micro- and nano-scale pores, where gases primarily adsorb. Consequently, comprehending gas adsorption mechanisms in shale nanopores is imperative for shale gas geological storage. In this study, we simulated CO₂, H₂S and CH₄ adsorption in organic/inorganic shale nanopores under various pressures using grand canonical Monte Carlo (GCMC) simulations. We calculated their adsorption quantities and selectivity coefficients under assorted conditions and analyzed competitive adsorption. This work elucidates shale gas adsorption from a molecular perspective and lends insights into storage assessments.

Methods/Procedures/Process:

We constructed molecular models of shale nanopores with diverse structures, encompassing hydroxylated quartz nanopores and graphitic organic nanopores. We examined CO₂, H₂S and CH₄ adsorption in these pores under various pressure conditions (373.15K). The molar ratio of CO₂, H₂S and CH₄ was fixed at 4:1:5. CLAYff and Steele 10-4-3 potential models described quartz and graphite correspondingly, while the TraPPE and Nath force field models represented CO₂/CH₄ and H₂S individually. Component densities and chemical potentials were computed based on gas composition. CO₂, H₂S and CH₄ insertions, translations and rotations were conducted over 20 million MC cycles, equalizing pore gas chemical potentials to calculated values. The first 12 million cycles achieved chemical potential equilibrium, and the subsequent 8 million cycles collected gas distribution data. The Langmuir-Freundlich adsorption model fitted the isotherms. Competitive gas adsorption was examined by quantifying adsorption quantities and selectivity coefficients.

Results/Observations/Conclusions:

Gas adsorption capacities were superior in organic versus inorganic pores across all gases examined. Graphite ostensibly furnished additional adsorption sites, whereas hydrogen sulfide and carbon dioxide occupied further sites in quartz nanopores. Therein, CH₄ adsorption selectivity was markedly inferior to CO₂ and H₂S. Excess CH₄ adsorption approached 0 as pressure rose, however excess CH₄ adsorption in organic pores increased with pressure. H₂S displayed the maximal adsorption selectivity coefficient universally, imprinting the strongest competitive adsorption capacity, which intensified in organic nanopores. Under certain quartz pore conditions, CO₂ adsorption selectivity closely approximated H₂S and exceeded CH₄ substantially, unveiling comparable CO₂ and H₂S competitive adsorption capacities in inorganic pores given natural gas presence in reservoirs.

Applications/Significance/Novelty: This study elucidates the competitive adsorption between acidic gases and natural gas in depleted shale gas reservoirs from a molecular vantage, thus facilitating augmented comprehension of CO₂/H₂S adsorption mechanisms in natural gas-laden formations while steering acidic gas geological storage in shale.

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Session Classification: MS13

Track Classification: (MS13) Fluids in Nanoporous Media