Modeling Partitioning of Fluid Mixtures in Shale Nanopores

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Over the past few years, production of shale gas and shale light-oil has been greatly increased with much more production projected for the coming decades. Unlike conventional hydrocarbon reservoirs, a significant portion of the light hydrocarbons produced from unconventional shale reservoirs originate from connected intra-particle organic-matter pores, and a significant portion of those pores can be tens of nanometers or less. The nanoconfinement of hydrocarbons can affect the phase behavior and partitioning of components between the matrix and production fractures due to various interactions between the fluid molecules and pore surface. Therefore, understanding the fluid mixture partitioning between the bulk phase and a confined space is of great importance for predicting the total hydrocarbon storage, optimizing gas injection, and determining the operating conditions. Here we report modeling the fluid adsorption and desorption in shale nanopores using a molecular density functional theory (iSAFT), with a focus on short alkanes and carbon dioxide (CO_2). Molecules are modeled as flexible chains with different numbers of spherical segments, and they interact with each other by Lennard-Jones potential. The interaction between pore surface and the fluid is modeled by two approaches. For impermeable graphite pores, it is implicitly included by an external potential (Steele 10-4-3 potential), and for permeable kerogen pores the interactions are explicitly accounted for by Lennard-Jones interactions. The fraction of recovery for each component from shale pores is characterized by their partitioning coefficients between bulk and pore, which is an indication of their individual preference to stay inside or outside the pores. We study the partitioning of mixtures of alkanes and alkanes with CO₂ under typical reservoir conditions. For an alkane mixture, the partitioning coefficients of heavy components decrease as the pressure increases, which results from the entropic penalty of adsorption. For CO₂ and light alkane mixtures, CO₂ has a larger partitioning coefficient, which explains the enhanced gas production from shale by CO₂ injection.