Monte Carlo simulation of interfacial properties of water and carbon dioxide under confinement

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Enhanced natural gas recovery needs a precise and realistic characterization of solid fluid interfacial properties. This fact is especially relevant when the case of tight gas reservoirs is considered, where the adsorption is very high and an external water based fluid is injected in the reservoir with the objective to modify the system interfacial properties improving extraction rates. Following previous results on confined methane, in this work a recent technique proposed to study interfacial properties using molecular simulation, the Test Area [1], has been used to determine the interfacial tension of water and carbon dioxide confined in slab geometry, composed by two parallel structureless interacting walls. These values have been compared with those obtained from the analysis of the pressure components inside the pore. Density profiles and adsorption coefficients have been calculated as well, considering the influence of wall spacing and testing several wall-fluid interaction potentials. Carbon dioxide has been modeled as a Lennard Jones sphere plus an isotropic multipolar (IMP) contribution [2]. In the case of water, the TIP4P-2005 model was considered, whose excellent comparative performance to describe water phase equilibria and thermophysical properties has been recently demonstrated [3].

References.

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