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Coarse-grained simulations of multiphase distribution in porous media, with application for oil and for gas hydrates

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Extraction of hydrocarbon fuels, including oil, gas and gas hydrates, often occurs from natural porous materials, such as shale, sands, or sediment, and as such is controlled by capillary interactions. The key consideration governing the effects of capillarity in porous materials is the spatial distribution and interplay of water, gas, and other phases within the pore space. The distribution of phases and corresponding interfaces determine the response to chemical, physical, and mechanical driving forces. Experimental determination of the phase distribution within a pore space is available via X-ray micro-computed tomography (microXCT). However, the phase distribution is difficult to predict given the complexity of the pore space geometry.

A coarse-grained Monte Carlo lattice simulation methodology was developed that allows determination of the spatial distribution of various components (e.g. air, water, oil, clathrate hydrate) within complicated pore space geometries. In many cases this geometry is obtained directly from experimental methods such as microXCT, where pore space geometry is discretized directly onto the simulation lattice. The methodology is applicable for pores on the nano through the macro scale. Constitutive properties of the pore system can be calculated, including soil-water retention, specific surface areas, and hysteresis. The methodology has been validated in simple geometries, and constitutive properties for complex systems such as Ottawa sand show excellent agreement with experiment. For multiple fluid phases, such as oil, water and air, we demonstrate how the various interfacial tensions can shift the effective composition of fluids as a function of pore size.

Biography

David T Wu is Professor of Chemistry and Chemical Engineering at the Colorado School of Mines, where he is Head of the Department of Chemistry and Geochemistry, and is Associate Director for the CSM Center for Hydrate Research. He received his PhD in Chemistry from the University of California at Berkeley and his BA in Chemistry from Harvard University. He carried out Postdoctoral studies in Physics at Cambridge University, and in Chemical Engineering at the University of California at Santa Barbara. His research focuses on physical chemical phenomena in hydrates, granular and porous materials, and theoretical and computational statistical mechanics.

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