Molecular modeling of gas adsorption and release from subsurface porous media

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Gas adsorption and release from subsurface porous media such as kerogen and clay aggregates play important roles in shale gas production, enhanced gas recovery, and carbon sequestration. In this work, we investigated the adsorption and release of CO_2 and CH_4 in kerogen. Our results suggest that kerogen adsorbs more CO_2 than CH_4 and that most of the generated CO_2 during kerogen maturation will only be released when the reservoir pressure decreases below supercritical pCO_2. We have also shown that CO_2 can displace much of the CH_4 trapped in kerogen, even when CH_4 release is blocked by water in the nanopores.

For the gas-clay aggregates system, we have built complex and realistic clay aggregates with interparticle pores and boundaries (Fig. 1). We report the use of this model to investigate the effect of dewatering on the micro-porosity of clay aggregates. The results suggest that slow dewatering will create more compact aggregates compared to fast dewatering. Our work provides a mechanistic understanding at the atomistic scale of the effects of compaction and drying on the structure and texture of clay aggregates.

Both our kerogen and clay studies advance the molecular simulation models used to investigate subsurface porous media-fluid interfaces from simple (i.e., slit-shape pores) to more complex systems that have a range of pore sizes and variable pore connectivity.

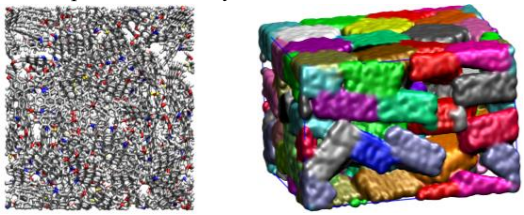

Fig 1. Simulation snapshot representing kerogen (left) and nanoparticle aggregate (right) with interparticle pores and boundaries obtained from our simulation. Each colour represents a particle.

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