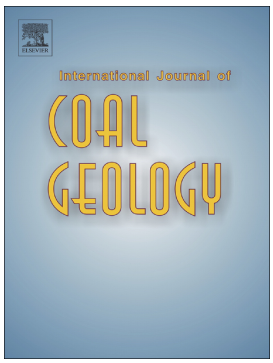

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Microstructure and adsorption properties of organic matter in Chinese Cambrian gas shale: Experimental characterization, molecular modeling and molecular simulation

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ABSTRACT

A representative molecular model of shale organic matter (OM) is prerequisite to further theoretic investigation on the fundamental mechanisms governing storage, transport and recovery of shale gas. In this work, a systematic strategy to prepare structural and compositional properties of OM is reported first, and then a realistic molecular model of Chinese Cambrian OM is generated based on analytical experimental data. Microstructure characterization and adsorption simulation are further performed using molecular dynamics simulation and grand canonical Monte Carlo simulations, respectively. The OM model, composed of kerogen macromolecules, bitumen components and residual lighter components, shows a reasonable representation of realistic Cambrian OM with respect to structural parameters, generic compositions, physical density and porosity. The OM porous network consists of dominant ultra-micropores and limited micropores. Compared with heavier components, lighter components are more inclined to occupy accessible pores. Interestingly, lighter components are observed to appear in pairs due to competitive adsorption around heteroatom groups. Water molecules are scattered in the system because of abundant functional groups and poor pore connectivity. The OM skeleton represents the adsorption behaviors of methane, carbon dioxide and nitrogen well. The adsorption capacity is carbon dioxide > methane > nitrogen. A higher adsorption capacity corresponds to a lower pressure when the excess isotherm reaches the maximum. The adsorption behaviors of heavier hydrocarbon species (ethane, propane and n-butane) cannot be represented in the OM skeleton with ultra-micropores and limited micropores, and the effect of molecular sizes of these species cannot be neglected. This work reports a systematic construction process for realistic molecular model of shale OM, and the representative OM model can serve as a starting point to explore gas adsorption and transport mechanism in shale organic pores at