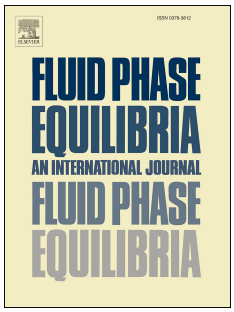

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Structural and Dynamical Properties of Methane Clathrate Hydrates from Molecular Dynamics: Comparison of Atomistic and More Coarse-Grained Potential Models

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In an attempt to study the accuracy and utility of 'coarse grained' models for methane-clathrate systems, molecular-dynamics simulations were run for three different potential models. One was fully atomistic of TIP4P water and fully atomistic methane, the next model was atomistic SPC water and coarse-grained UA methane, whilst the final model was the fully coursed-grained mW model. All models were run at two different sizes (8 and 64 fully-occupied sI clathrate unit cells) at 250 K and 60 bar. It was found that the coarse-grained models had a high level of accuracy in recreating structural properties, such as density or radial distribution functions (RDFs), with the obvious exception of not being able to create RDFs for atoms which are neglected by the model. More coarse grained models were shown to have lower accuracy for time-dependent phenomena, such as identifying the density or velocity fluctuations' frequencies.

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