

Application of the TraPPE force field to predicting isothermal pressure-volume curves at high pressures and high temperatures¹

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ABSTRACT

Knowledge of the thermophysical properties of materials at extreme pressure and temperature conditions is essential for improving our understanding of many planetary and detonation processes. Significant gaps in what is known about the behavior of materials at high density and high temperature exist, largely due to the limitations and dangers of performing experiments at the necessary extreme conditions. Modelling these systems through the use of equations of state and particle-based simulation methods significantly extends the range of pressures and temperatures that can be safely studied. The reliability of such calculations depends on the accuracy of the models used. Here we present an assessment of the united-atom version of the TraPPE (Transferable Potentials for Phase Equilibria) force field and single-site exp-6 representations for methane, methanol, oxygen, and ammonia at extreme conditions. As shown by Monte Carlo simulations in the isobaric-isothermal ensemble, the TraPPE models, despite being parameterized to the vapor-liquid coexistence curve (i.e. relatively mild conditions), perform remarkably well in the high pressure/high temperature regime. The single-site exp-6 models can fit experimental data in the high pressure/temperature regime very well, but the parameters are less transferable to ambient conditions.