

# Simulating vapor-liquid nucleation in n-alkanes

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## Abstract

A combination of the aggregation-volume-bias Monte Carlo algorithm, the configurational-bias Monte Carlo algorithm, and the umbrella sampling technique was applied to investigate homogeneous vapor-liquid nucleation in ethane, n-butane, and n-heptane. The simple TraPPE-UA force field was used in this investigation. It was found that for the n-heptane case, the TraPPE-UA force field predicted a nucleation rate that is about 3-4 orders of magnitude higher than that measured by an upward thermal diffusion cloud chamber experiment. Comparison of the simulation results to the classical nucleation theory (CNT) shows that CNT consistently overestimates the barrier heights for all chain lengths investigated. The offset on the barrier heights was found nearly independent of the supersaturation for both ethane and n-butane, similar to a Lennard-Jonesium system previously studied. This also directly leads to a good agreement on the cluster sizes between the simulation and the CNT calculated from the nucleation theorem. For n-heptane, however, the offset was found dependent on the supersaturation. It appears that CNT predicts a slightly weaker dependence of the nucleation rate on supersaturation, which agrees with both density functional calculations and the experiments.

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