Computer Simulations, Nucleation Rate Predictions and Scaling
BARBARA HALE, University of Missouri-Rolla — Computer simulations which generate small molecular cluster size distributions for use in steady state nucleation rate predictions and direct molecular dynamics simulations of the nucleation process depend crucially on the properties of the effective pair potentials and on the modeled system’s metastable conditions. The latter conditions often differ significantly from those under which the experimental data are taken. For argon, in particular, simulations using both truncated and full Lennard-Jones potentials have generated a range of results for the nucleation rate, \( J \), which, in magnitude, appear to be inconsistent with the limited experimental rate data. We propose that \( \log J \) should be plotted versus a “universal” function of the scaled supersaturation, \( \ln S/[(T_c/T – 1)^{3/2}] \), which incorporates scaling of metastable system conditions with potential model (or experimental) properties, as appropriate. This plot, which provides a more realistic comparison of predicted and experimental rates, is applied to water and to argon data. For argon, this plot emphasizes the limited range of simulation results at large scaled supersaturations and suggests that none of these predicted rates are inconsistent with the much smaller experimental nucleation rates taken at reduced scaled supersaturations. For water, the plot indicates that experimental nucleation rates are likewise well characterized by the scaled supersaturation function.