

Abstract Submitted  
for the MAR11 Meeting of  
The American Physical Society

**Scaling of Nonclassical Nucleation Rates of Methanol** GERALD WILEMSKI, FAWAZ HRAHSHEH, Missouri University of Science and Technology, Rolla MO, ABDALLA OBEIDAT, Jordan University of Science & Technology, Irbid, Jordan — Nonclassical gradient theory (GT) calculations of nucleation rates are presented for methanol, an associating vapor system. The calculations use the SAFT-0 equation of state (EOS) that accounts for the effects of molecular association based on the statistical association fluid theory (SAFT). Calculated rates were compared to the experimental rates of Strey, et al. [*J. Chem. Phys.* **1986**, 84, 2325]. The GT nucleation rates showed improved  $T$  and  $S$  dependence compared to classical nucleation theory (CNT). The GT rates were also improved by factors of 100-1000 compared to CNT. Despite these improvements, GT does not describe the reported  $T$  and  $S$  dependence of the nucleation rates. To explore this further, the GT and experimental rates were analyzed using Hale's scaled model [*J. Chem. Phys.* **2005**, 122, 204509]. This analysis reveals an inconsistency between the predictions of GT, which scale relatively well, and the experimental data, which do not scale. It also shows that the measured rate data have an anomalous  $T$  and  $S$  dependence. A likely source of this anomaly is the inadequate thermodynamic data base for small cluster properties that was used originally to correct the raw rate data for the effects of association.

Gerald Wilemski  
Missouri University of Science and Technology, Rolla MO

Date submitted: 24 Nov 2010

Electronic form version 1.4