Nucleation of Multicomponent Droplets

Ailo Aasen [C, S]
Norwegian University of Science and Technology, Trondheim, Sør-Trøndelag, Norway
ailo.aasen@ntnu.no

Øivind Wilhelmsen
Norwegian University of Science and Technology, Department of Energy and Process Engineering, Trondheim, Norway
SINTEF Energy, Department of Gas Technology, Trondheim, Norway

Classical Nucleation Theory (CNT) models the Gibbs free energy of a nucleating droplet as the sum of a negative contribution from the bulk fluid that is proportional to the volume of the droplet, and a positive contribution that equals the surface tension times the droplets area. The critical cluster corresponds to a maximum of the Gibbs free energy. One of the most questionable assumptions in CNT is that the critical cluster has the same surface tension as the flat surface. In reality, surface tension depends on interfacial curvature. Curvature corrections for the surface tension become especially relevant for the small droplet sizes considered in CNT, and may account for part of the discrepancy between the experimental results, simulations, and theory. A simple approach to incorporate this dependence into CNT has previously been investigated for pure water [1]. This approach was shown to correct most of the erroneous temperature dependence of nucleation rates from CNT. Using a newly developed framework for curvature corrections for multicomponent droplets [2], we present an extension of nucleation theory to mixtures which, for the first time, incorporates the curvature dependence of the surface tension. We evaluate the effects this has on the prediction of nucleation rates for a real binary system.

References:

[1]. Ø. Wilhelmsen, D. Bedeaux and D. Reguera (2015). Tolman length and rigidity constants of water and their role in nucleation. *Journal of Chemical Physics* 142 (17), doi: 10.1063/1.4919689.
[2]. A. Aasen, E.M. Blokhuis and Ø. Wilhelmsen (2018). Tolman lengths and rigidity constants for multicomponent systems: Fundamental theory and numerical examples. *To be submitted*.