Thermophysical Properties from Nucleation Simulations

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Abstract

Classical Nucleation Theory (CNT) has been a dominant model in understanding the self-assembly of new thermodynamic phases, whose initial step involves the growth of embryos in a metastable environment. This provides significant explanations to thermodynamic processes including thin film condensation and crystallization of liquid alloys among others. Surface tension property is critical in understanding the formation of aerosols and other nucleating substances. Calculation of this property both from the theoretical and experimental perspective is rather tedious and inexact. This work investigates the possibility of deriving a surface tension value from simply performing a density measurement. Also, this work will reevaluate existing surface tension – temperature equations. Results may provide better means of calculating surface tension of any liquid at any temperature without performing additional experiments. In this ongoing study, the energy profiles of nine compounds (1-pentanol, 1-hexanol, 1-heptanol, pentane, hexane, heptane, butanoic acid, pentanoic acid, and hexanoic acid) at five temperatures are obtained using Aggregation-Volume-bias Monte Carlo simulation.

Methods

Simulations will be done for 25 neat liquids and 5 binary mixtures at 5 different temperatures. Based on similar systems that have been studied previously, simulations of neat liquids will require approximately 1000 SUs for production and 4000 SUs to converge the bias potential which is usually done on 8-16 processors for unary systems. 1SU = 1 processor-hour

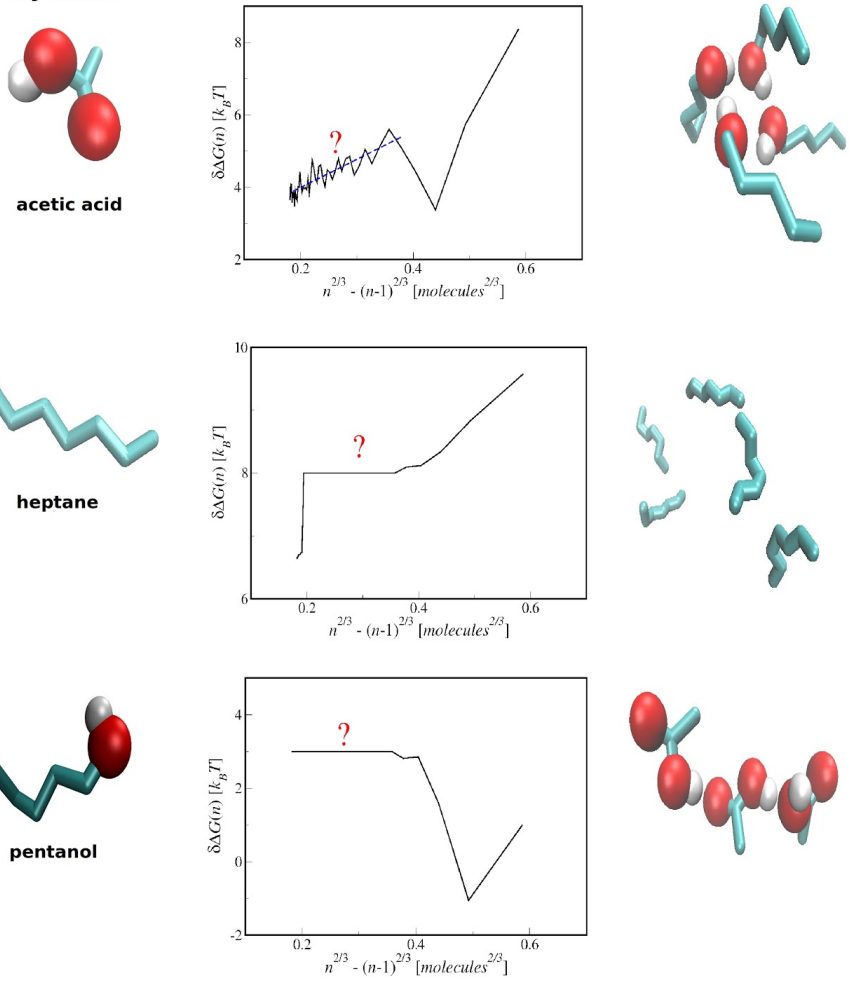
(1000 SUs production + 4000 SUs convergence) x 25 neat liquids x 5 temperatures = 625,000 SUs

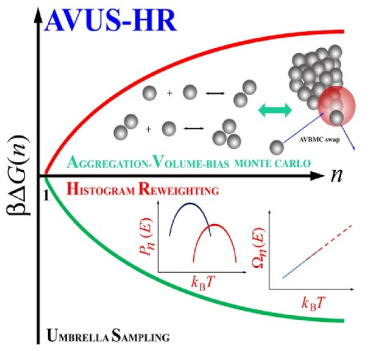
For binary mixtures the costs will be increased as discussed above due to the need to sample n^2 points where n is the number of molecules of each component. For these systems, production will require 5000 SUs and the bias potential convergence will require about 10,000 SU.

(5000 SUs production + 10,000 SUs convergence) x 5 mixtures x 5 temperatures = 375,000 SUs

Once the free energy profiles of the different systems in this study are obtained, the unknown properties can be derived.

Systems





Conclusion

The data we have at the moment, although insufficient to arrive at a concluding point, show promising features.

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