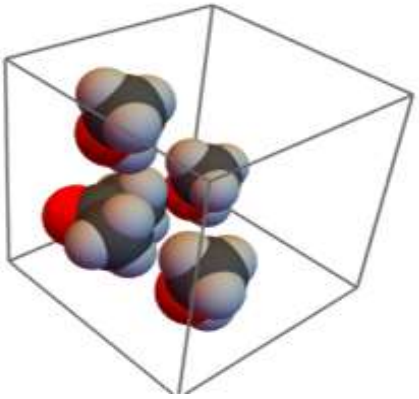
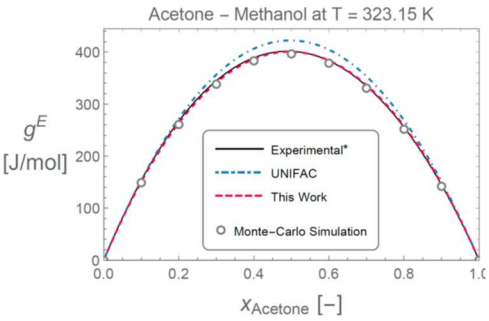
Activity Coefficient Model Refinement

Topic suitable for Master Thesis / Plant Design

A recently published thermodynamic model [1] is based on variables that describe clusters of four molecules, as shown in the figure. To provide parameters for this model, the molecules of the cluster are arranged in a random way, and the energy of such a cluster 'sample' is calculated with a molecular force field. This algorithm is implemented in Wolfram Mathematica [2].



The goal of this work is to apply this Mathematica notebook for sampling selected two-component systems, to use the samples as input for the thermodynamic model and to compare the results of the model with experimental data. Based on this comparison, the sampling strategy shall be enhanced to further increase the model performance.



For operating the well-documented sampling package, a basic understanding of Wolfram Mathematica concepts is required, e.g., by exploring the interactive website http://www.wolfram.com/wolfram-u/an-elementary-introduction-to-the-wolfram-language/.

Literature:

[1] Mayer C, Wallek T: https://doi.org/10.3390/e22101111

[2] Steiner T: MSc-thesis 2019, Graz University of Technology

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