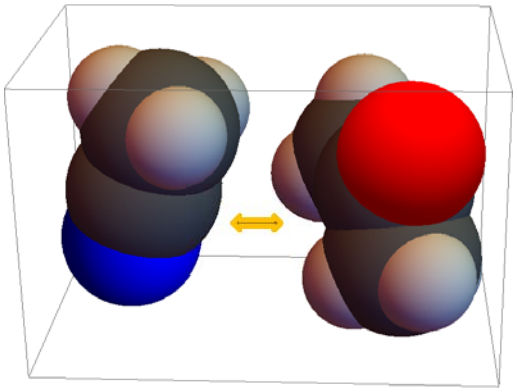
Graz University of Technology
Institute of Chemical Engineering and Environmental Technology
Plant and Process Design & Chemical Engineering Thermodynamics

☒ Bachelor's thesis
☒ Plant design exercise
☐ Paid master's thesis
☒ Computational
☐ Experimental
☐ Plant design related

Application & Enhancement of a Molecular Sampling Algorithm

A recently published thermodynamic model [1] is based on variables that describe clusters of molecules. In the easiest case, such clusters consist of two molecules, as shown in the figure. To provide variables for the model, the molecules of the cluster are arranged in a random way, and the energy of such a cluster 'sample' is calculated using a molecular force field. This algorithm is already implemented as a Wolfram Mathematica program [2]. The goal of this work is to apply the algorithm to sampling of selected molecules, to use these samples as input for the thermodynamic model and to enhance the sampling strategy gradually by comparing the results of the model with experimental data.



A basic knowledge of Wolfram Mathematica concepts is required, e.g. by exploring the interactive elementary introduction http://www.wolfram.com/wolfram-u/an-elementary-introduction-to-the-wolfram-language/

The thesis can be written in either *English* or *German*.

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Literature: [1] Wallek, Mayer, Pfennig: Ind. Eng. Chem. Res. 2018, 57, 1294-1306.

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