Calculation of interfacial tension

The interfacial tension ("21Interfacial tension" in the MoDeNa workflow) is passed from tool "3WP1 Thermo tools DFT (US)" to "11WP3 CFD tool (POLITO)", "13WP3 Rheology tool (TUE)", "6WP2 Bubble growth tool (VSCHT)", "10WP2 wall drainage and rupture tool (VSCHT)" and "7WP2 Coalescence Kernel tool (TUE)".

The final input parameters of the model call will be temperature, pressure and composition and the value of interfacial tension as the output parameter. The call as of now only has temperature as input and interfacial tension as output. This is because the influence of pressure is usally small and is neglected in this first version of the surrogate model and furthermore it is still undecided how to specify composition.
Furthermore, the PC-SAFT parameters of the actual PU polymer have not been determined yet. For now the model returns the surface tension (in $^{\mathrm{mN}}/_{\mathrm{m}}$) at the specified temperature of the simple system octane-argon at a pressure of 1.013 bar.

To compile the code of the detailed model, PETSc-3.4.4 needs to be installed. A makefile is included.

Detailed Model

As the detailed model a density functional theory code based on the PC-SAFT equation of state is used. Please see [1] for the underlying theory and comparisons to experimental results.

The code reads the temperature (in K) at which to calculate the interfacial tension from the input file *in.txt* and writes the calculated interfacial tension to the output file *out.txt*

Surrogate Model

The interfacial tension decreases with increasing temperature and vanishes at the critical point. It is often valid to assume that this temperature denpendence is close to linear [2]. Furthermore, as long as pressure values do not change substantially, the influence of pressure on the interfacial tension is small.
Figure 1 shows this linear temperature dependence and the influence of pressure for the system octane-argon.

Therefore, a simple linear equation is used as a surrogate model for the interfacial tension γ:

$\gamma(T) = A + B \cdot T$

However, should more realistic systems of the MoDeNa project exibit pressure influences which cannot be neglected, this pressure dependence can easily be captured by a more sophisticated surrogate model.

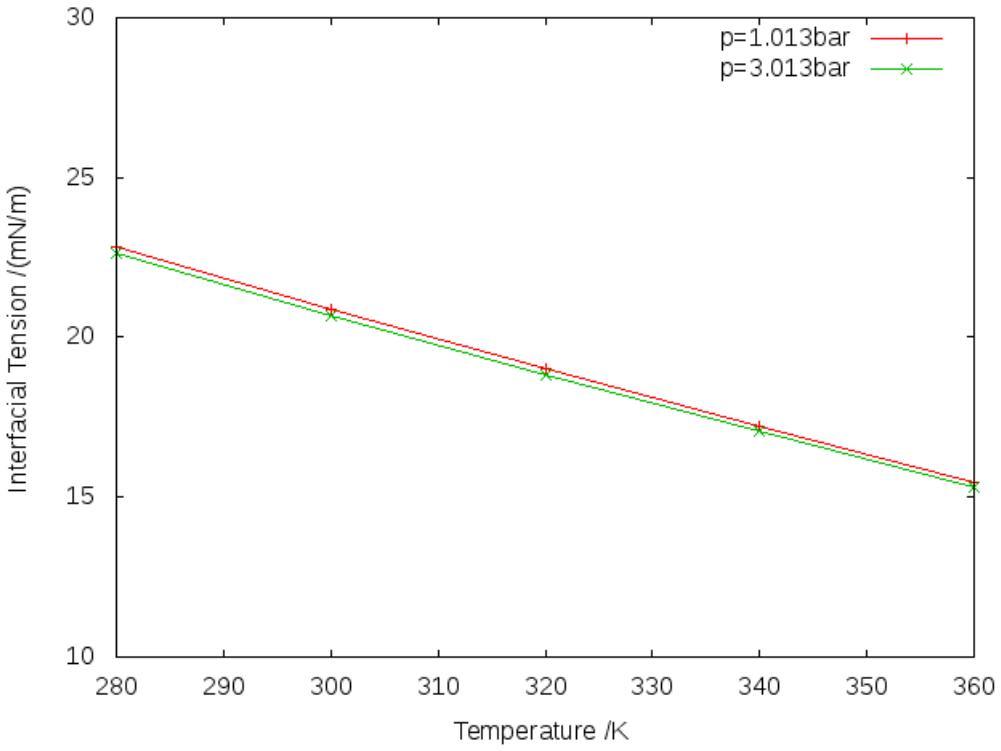

Figure 1: Interfacial tension of the system octane-argon at different temperatures and pressures.

Design of experiments

As soon as the surrogate model is called to evaluate the interfacial tension for a temperature value outside the temperature range it was fitted for, the detailed model is called to provide a new data point. This new data point is chosen to be 10% larger (smaller) than the requested value if this requested value is above (below) the current temperature intervall that was used to fit the parameters of the surrogate model.

Bibliography

[1] J. Gross. A density functional theory for vapor-liquid interfaces using the pcp-saft equation of state. *The Journal of Chemical Physics*, 131(20):–, 2009.

[2] B. Pohling, J. Prausnitz, and J. O'Connell. *The Properties of Gases and Liquids*. McGraw-Hill, 2001.