Calculation of Polymer Density

The density ("7Bulk density of Polymer" in the MoDeNa workflow) is passed from "4WP1 Thermo Tools (US)" to "11WP3 CFD Tool (POLITO)" and "6WP2 Bubble Growth Tool (VSCHT)".

This model is called from systems where the compositions of the liquid phase is known (either because only the polymer is present, e.g. in the case of POLITO or because the composition has been obtained in a different way before this model call, e.g. in the case of VSCHT).
Therefore, this model returns the density of the liquid phase rather than the density of only the polymer. With the known molar or mass fractions of the components in the liquid phase, the polymer density can then easily be obtained from this liquid phase density.
The final call to the model will have temperature and a variable specifying which other components besides the polymer are present in the system as input parameters and the density of the liquid phase as the output value.
As it is still undecided how to identify components, the call as of now only has temperature as input and the density as output.
Furthermore, because the PC-SAFT parameters of the actual PU polymer have not been determined yet, a model system is studied here containing a polyethylene with a molecular mass of $1000 g/mol$ as well as pentane and carbon dioxide as examples of a physical and a chemical blowing agent, respectively.

The value of pressure is set to $p = 1.013$bar in all simulations.

Detailed Model

As the detailed model the PC-SAFT equation of state is used. Please see [1], [2] and [3] for the underlying theory and comparisons to experimental results.

The code reads the temperature at which to calculate the density from the file *in.txt*. It then calculates the phase equilibrium at this temperature and a pressure of $p = 1.013$bar.

The value of the density of the liquid phase (in kg/m^3) is then written to the output file *out.txt*.

Surrogate Model

As the surrogate model, we use a modified Rackett equation which is usually fit to experimental values of liquid densities [4]. Here we fit the equation to results of the PC-SAFT equation of state. The Rackett equation reads:

$$\rho = \frac{A}{B^{(1+(1-T/C)^D)}}$$

where A,B,C and D are fittable parameters and T denotes temperature in Kelvin.
To avoid problems in the fitting procedure, D is set to 1 here. As figure 1 shows, the surrogate

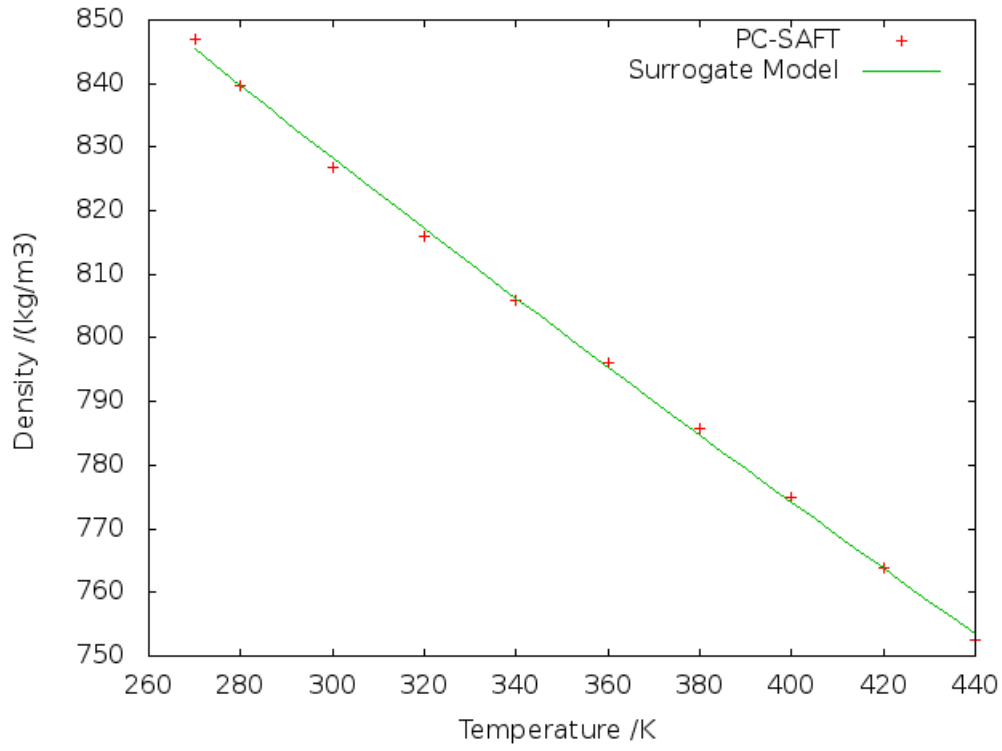model still reproduces the density values of the detailed model very well.

Figure 1: Density of the liquid phase as calculated with the PC-SAFT equation of state and the surrogate model.

Design of experiments

As soon as the surrogate model is called to evaluate the Henry coefficient 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 and G. Sadowski, "Perturbed-chain saft: an equation of state based on a perturbation theory for chain molecules," *Industrial & Engineering Chemistry Research*, vol. 40, no. 4, pp. 1244–1260, 2001.

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[3] J. Gross and J. Vrabec, "An equation-of-state contribution for polar components: Dipolar molecules," *AIChE Journal*, vol. 52, no. 3, pp. 1194–1204, 2006.

[4] V. D. Ingenieure, *VDI-Waermeatlas -*. Berlin, Heidelberg: Springer, 10. aufl. 2006 ed.