The GC-PPC-SAFT within ProSim : an industrially relevant tool

Jean-Charles de Hemptinne [a, †], J-P Passarello, R. Lugo, N. Ferrando, S. Massebeuf, O. Baudouin

[a] IFP Energies nouvelles, 1-4 avenue de Bois-Préau, Rueil-Malmaison 92852, France

[†] E-mail: j-charles.de-hemptinne@ifpen.fr

Abstract

The SAFT equation of state is now widely known in the thermodynamic research community. Its qualities are essentially its predictive power as it takes into account explicitly the main intermolecular interactions (repulsion, van der Waals forces, hydrogen bonding, polarity). The group contribution approach makes it possible to investigate in a predictive manner a large set of compounds (as illustrated by Nguyen, T.B.).

Yet, it has not, to our knowledge, been applied to an industrial process. This presentation aims at showing the capacity and limitations of the method through some examples that we have been involved with:

- Ethanol dehydration using n-butane
- Solvent evaluation for supercritical biomass pyrolysis process
- Ethanol to Ethylene

The main learnings from these case-studies are that the close collaboration with a software vendor allows for a better understanding of the needs of the process engineer, and more specifically related to computation time.

Keywords: Group Contribution, GC-PPC-SAFT, binary interaction parameter, LLE, oxygenated compounds.