Ethanol Dehydration Process Simulation with GC-PPC-SAFT

O. Baudouin [a*], S. Déchelotte [a], N. Ferrando [b], J-C. de Hemptinne [b], R. Lugo [b], S. Massebeuf [a]

[a] ProSim, Stratège Bâtiment A, 51 rue Ampère, 31670 Labège
[b] IFP Energies nouvelles, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison

[*] Corresponding author, Tel.: +33562882440, fax: +33562882439, E-mail: Olivier.baudouin@prosim.net

The MEMOBIOL (Modélisation à l'Echelle MOléculaire pour les BIOraffineries Lignocellulosiques - Molecular Scale Modeling for Lignocellulosic Biorefineries) project, led by IFPEN, focusing on molecular modeling applied to lignocellulosic biomass (wood residues, cereal straw, forestry waste) has been selected by the ANR (French National Research Agency, ANR-09-CP2D-10-01) as part of its 2009 "Chemistry and Processes for Sustainable Development" call for projects. In addition to IFPEN, the project brings together six partners from the academic world (Armines -École des Mines de Paris CEP/TEP-, ENSTA-ParisTech -École Nationale Supérieure des Techniques Avancées- and LSPM - Laboratoire des Sciences des Procédés et des Matériaux-), and the industry (Materials Design and ProSim).

Lignocellulosic biomass is likely to play a major role as a substitution material in the chemicals sector. When designing new chemical products and manufacturing processes using lignocellulosic matter, chemistry needs to have access to tools able to characterize the molecules associated with the conversion of these bio-resources. MEMOBIOL therefore aims to develop new modeling and calculation technologies capable of modelling the physicochemical behavior of molecules derived from lignocellulosic biomass (phase equilibria in particular). Unlike hydrocarbons, these molecules belong to a variety of complex oxygen-containing families that feature polar and associative character. These physical phenomena must be explicitly taken into account in the modelling tools.

Within the framework of this project, "conventional" modelling tools based on the use of an equation of state (GC-PPC-SAFT), on which IFPEN and LSPM have been working together closely for several years already [1-4], was developed. This model is made available to industry in the thermophysical calculation server Simulis® Thermodynamics, marketed by ProSim. It is noteworthy that thanks to its implementation of the CAPE-OPEN standardized interfaces, GC-PPC-SAFT can be used in any CAPE-OPEN compliant. This predictive equation of state was used to model, with the general steady state process simulator ProSimPlus®, an ethanol dehydration process using n-Butane as entrainer. Comparisons were performed with experimental data and other predictive models available in Simulis® Thermodynamics (UNIFAC[6], PSRK[7]).

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