Using SAFT for Lignocellulosic Biorefineries Modeling

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MEMOBIOL project overview

The MEMOBIOL (Modélisation à l'Echelle MOléculaire pour les BIOraffineries Lignocellulosiques - Molecular Scale Modeling for Lignocellulosic Biorefineries) project, 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 (visit the web site for more information: http://projet.ifpen.fr/Project/jcms/xnt_10367/memobiol).

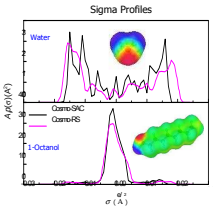
Lignocellulosic biomass is likely to play a major role as a substitution material in the chemicals sector. When designing new chemical products and manufacturing processes using lignocellulosic matter, chemistry needs to have access to tools capable of characterizing the molecules associated with the conversion of these bio-resources. MEMOBIOL therefore aims to develop new modeling and calculation technologies capable of reconstructing the physicochemical behavior of molecules resulting 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 modeling tools.

The project brings together six partners from the academic world (Mines ParisTech -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 (IFPEN, Materials Design and ProSim).

MEMOBIOL organization

COSMO methods. Parameterization of classical models (e.g. UNIQUAC, NRTL) from ab initio calculations

Ensta-Paristech



Binary Interaction Parameters

ProSim

Simulis® Thermodynamics

Models integration for industrialization (**Process simulation**)

Models, Parameters

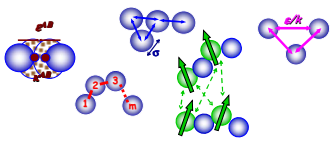
Mines ParisTech

Models **experimental** validation

Experimental data

GC-PPC-SAFT Eos development & parameterization

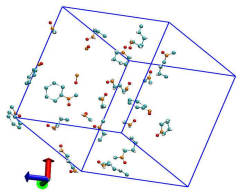
LSPM, Ensta-Paristech, IFPEN



$$\frac{A - A^{\circ}}{NkT} = m\left(a^{hs} + a^{disp}\right) + a^{assoc} + a^{chain}$$

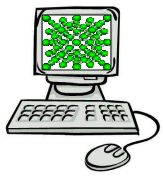
Pseudo-experimental data

Molecular simulation. Force field and Monte Carlo algorithms development for prediction of systems with oxygenated compounds



IFPEN

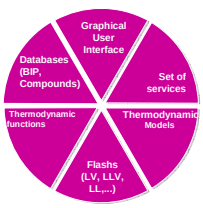
Algorithms, force fields



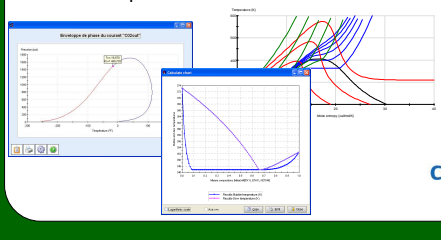
MedeA-Gibbs (Materials Design)

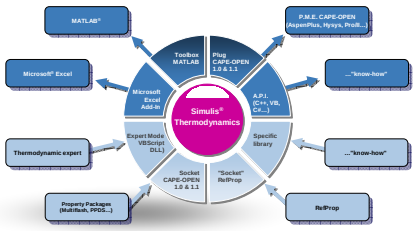
Models integration for industrialization (**Force fields, algorithm**)

Simulis® Thermodynamics



A complete thermodynamic calculation server, based on a software component architecture

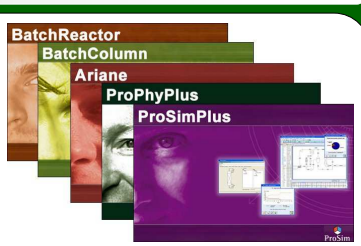


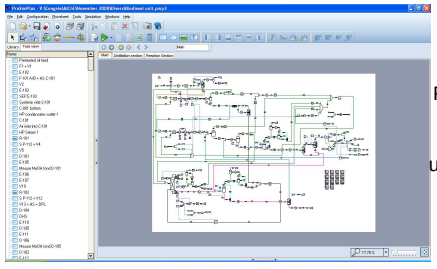


Can be embedded in any environment and really open to welcome user's specific know-how

Any application that integrates Simulis® Thermodynamics automatically inherits from its CAPE-OPEN standard compliance

Thermodynamic calculation server of all ProSim software (consistency between applications is automatically ensured)





ProSimPlus (Steady State Simulation Software) will be used for biorefineries simulation