MEMOBIOL

Modélisation à l'Echelle MOléculaire pour les BIOraffineries Lignocellulosiques*

*Molecular-based models for lignocellulosic biorefineries

CP2D 2009

Objective

The main objective of the MEMOBIOL project (2009 – 2013) is to evaluate different predictive tools for calculating the thermodynamic phase equilibria and the properties required by the chemical industry for the design of new chemicals and processes involved in the conversion of the lignocellulosic raw material.

Main Deliverables

- **STI deliverables (reports, publications, conferences)**
  - Evaluation of existing predictive thermodynamic models
  - Development of new models
- **Databases**
  - Inventory of available experimental data for high-value oxygenated molecules and their mixtures
  - New experimental data for high-value oxygenated compounds
  - New molecular parameters / descriptions for existing models
- **Software**
  - New release of Simulis® Thermodynamics providing the new PPC-SAFT EOS
  - New release of MedeA-Gibbs® with new functionalities

Partners

ProSim

ifp Energies nouvelles

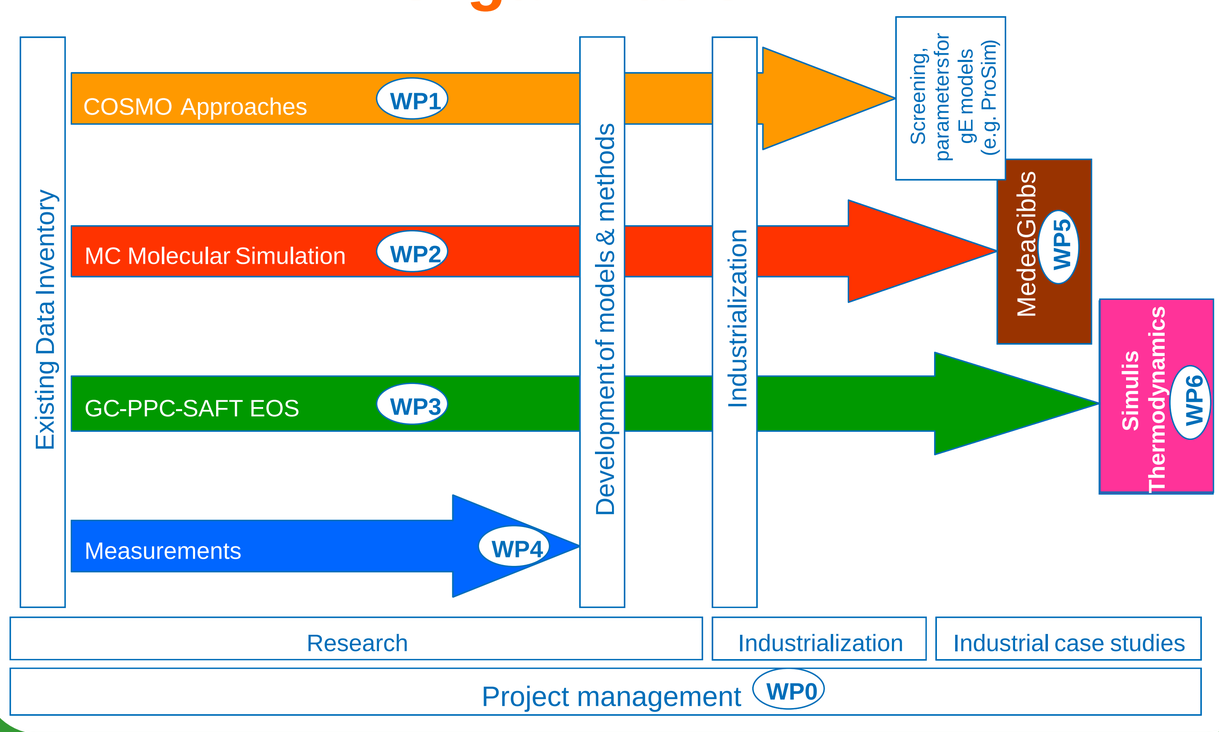
ENSTA ParisTech

materials design

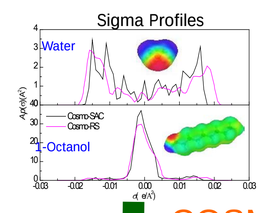
MINES PARIS

LSPM

Organization

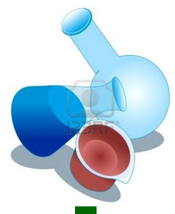


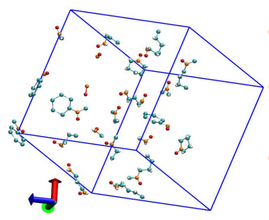
Technical scope



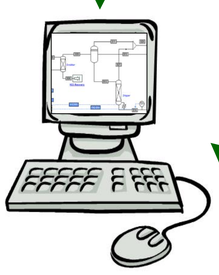
COSMO:
COnductor-like
Screening MOdel

Experimental measurements



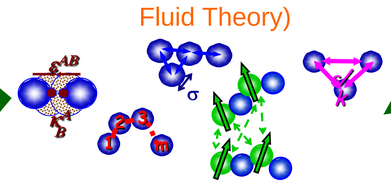


Molecular Simulation

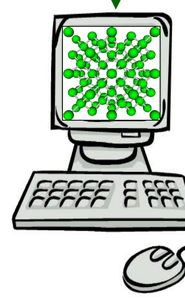


Process simulation software

SAFT EOS
(Statistical Associating Fluid Theory)

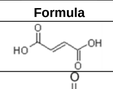
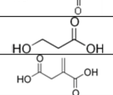
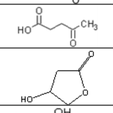
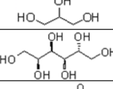
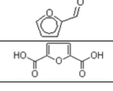


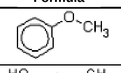
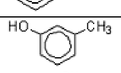
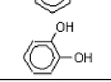
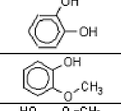
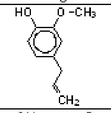
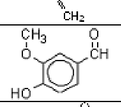
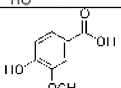
$$A^{res} = A^{hc} + A^{disp} + A^{chain} + A^{assoc} + A^{multi-polar}$$



Molecular Simulation Software

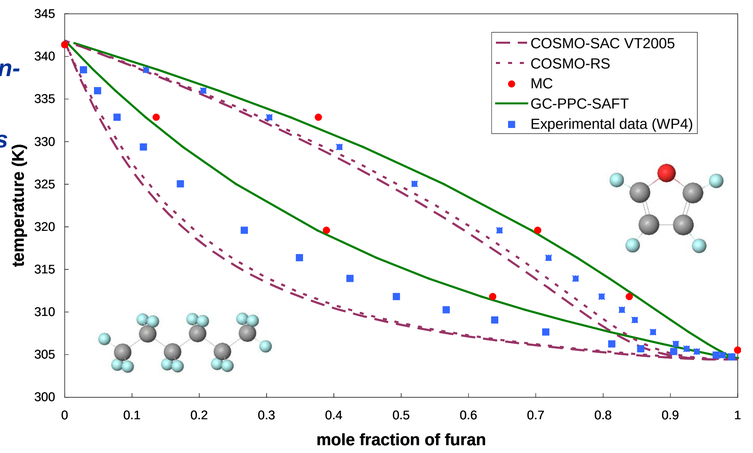
Molecules

Name	Formula
Fumaric acid	
3-hydroxypropionic acid	
Itaconic acid	
Levulinic acid	
3-hydroxybutyrolactone	
Glycerol	
Sorbitol	
Furfural	
2,5 furane dicarboxylic acid	

Name	Formula
Anisol	
m-Cresol	
Catechol	
Guaiacol	
Eugenol	
Vanillin	
Vanilic acid	
Quinone	
Syringol	

Main Results

- ✓ ***A thorough evaluation and comparison of COSMO-SAC and COSMO-RS approaches in the context of multifounctionnal oxygen-bearing molecules***
- ✓ ***An extension of the AUA4 force field to furans and organic acids***
- ✓ ***A thorough evaluation of the AUA4 force field to reproduce VLE/LLE of oxygenated molecules via Monte Carlo Molecular Simulation and a comparison with other force fields***
- ✓ ***Good prediction of hydrogen solubility in oxygean-bearing solvents using Monte Carlo Molecular Simulation***
- ✓ ***Recommendations on the most convenient frequencies for the different Monte Carlo moves***
- ✓ ***An evaluation of the use of the group contribution PPC-SAFT equation to reproduce VLE/LLE of oxygenated molecules***
- ✓ ***A new version of the associating term in the SAFT theory for acid-like association***
- ✓ ***New and original VLE/LLE/SLE experimental data for different binary and ternary systems containing high added-value oxygenated molecules and different solvents***



Reproduction of VLE of furan+n-hexane at 0.1 MPa using different predictive approaches. Experimental data have been obtained during the MEMOBIOL project.

Publications & Communications

Publications

- M. Nala, E. Auger; I. Gedik; N. Ferrando, M. Dicko, P. Paricaud, F. Volle, JP. Passarello, JC. de Hemptinne, P. Tobaly, P. Stringari; C. Coquelet; D. Ramjugernath; P. Naidoo, R. Lugo. Vapour Liquid Equilibrium (VLE) for the Systems Furan + n-Hexane and Furan + Toluene. Measurements, data treatment and modelling using molecular models. Fluid Phase Equilibria [Accepted]
- D. Fan, J. Li, J. shi, C. Peng, H. Liu, Y. Hu, P. Paricaud. Vapor-Liquid Equilibria in the Propyl Acetate þ Ethanoic Acid Binary System from (323.15 to 353.15) K: Measurement with a Static Method and Modeling with the NRTL, Wilson, UNIQUAC, and COSMO-SAC Approaches. Journal of Chemical Engineering Data. 56, 1323–1329, 2011.
- J. Li, P. Paricaud. Application of the COSMO-RS and COSMO-SAC model for the predictions of partition coefficients, vapor-liquid and liquid-liquid equilibria of bio-oil related mixtures. Energy & Fuels. DOI: 10.1021/ef300181j. 2012.

Oral communications

E. Auger, P. Tobaly, F. Volle, J-P. Passarello, M. Dicko. Determination of non-bonded fractions in a series of alkanols by spectroscopy. Influence on SAFT parameters. Esat (Postdam, 7-10 October 2012).
- R. Lugo. Predicting phase equilibria of oxygenated compounds using molecular models. Results from the MEMOBIOL project. InMoTher (Lyon, France). March 2012.
- J. Li, P. Paricaud. Prediction of the phase equilibria of mixtures with COSMO-like approaches: application to molecules extracted from bio-oils. Journée SFGP, Nancy, 2011.
- M. Yiannourakou, Ph. Ungerer, P. Saxe, B. Leblanc. H2 solubility in oxygen bearing compounds A Monte Carlo Study. Thermodynamics 2011, Athens, Greece.
- E. Auger, P. Tobaly, J.-P. Passarello and F.Volle. Spectroscopic investigation of hydrogen bonding in pure ethanol and ester + ethanol mixtures. Application to SAFT modelling Thermodynamics 2011 (September 1 – September3 / Athens / Greece)
- Marianna Yiannourakou, Philippe Ungerer, Benoit Leblanc and Paul W. Saxe. Monte Carlo Simulation of Fluid Phase Equilibria and of Adsorption In Microporous Materials : Investigation of Binary and Multicomponent Systems of Industrial Interest. 2011 AIChE – Annual Meeting (October 16 – October 21 / Minneapolis, MN / USA)

Posters

- M. Yiannoiurakou, M. Entrialgo-Castano,D. Rigby, B. Leblanc, N. Ferrando, P. Ungerer. Combined use of Molecular Dynamics and Monte Carlo simulations for the prediction of thermophysical properties , using All-Atom and United-Atom Forcefields. Fundamentals of Molecular Modelling and simulation (FOMMS), July 22-27, 2012, Oregon (USA).
- E. Auger, F. Volle, J-P. Passarello, P. Tobaly, J-C. de Hemptinne and R. Lugo. Modeling Phase Equilibria of Multifunctional Compounds of Interest for Biofuels Using GC-PPC-SAFT. SAFT 2010, Barcelona, Spain.
- Auger E., Passarello J.P., Paricaud P., Tobaly P., Volle F. Including polarizability effects in GC-PPC-SAFT: application to alkyl-ether containing systems. Esat 2011, Saint-Petersbourg, Russia.
- R. Lugo, N. Ferrando, J-C. de Hemptinne. C. Coquelet. P. Paricaud. P. Tobaly, J-P. Passarello, E. Auger, F. Volle. Ph. Ungerer, M. Yiannourakou, O. Baudouin. Le projet MEMOBIOL. Forum des groupes IEP et Thermo de la SFGP. Ensiacet (Toulouse), 12 mai 2011.
- Eric Auger, Pascal Tobaly, Fabien Volle , Jean-Philippe Passarello. Spectroscopic investigation of hydrogen bonding in associating compounds and mixtures. Application to SAFT Modelling. SAFT 2011 Discussion Meeting October 24-25, 2011, Pau, France.
- O. Baudouin, S. Massebeuf. E. Auger, J-P. Passarello, P. Tobaly, F. Volle., R. Lugo, N. Ferrando, J-C. de Hemptinne., C. Coquelet., P. Paricaud. Using SAFT for Lignocellulosic Biorefineries Modeling. SAFT 2011 Discussion Meeting October 24-25, 2011, Pau, France.
- J. Janecek, P. Paricaud. The influence of the Association Term on the behaviour of vapour phase of carboxylic acids. InMoTher (Lyon, France). March 2012.

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