THERMODYNAMICS PREDICTION FOR SEPARATING FLUIDS

Distillation and extraction are among the most important separation techniques in the chemical industry. The efficiency of the distillation depends on the difference in the equilibrium composition of the liquid and vapour phases. Therefore, distillation processes can only be designed if the vapour-liquid balance is known. The thermodynamic properties of fluids and solutions such as phase diagrams are predicted by a robust quantum chemical calculation-based COSMO-RS method. This method can be also applied to systems having no parameters or poorly represented in empirical models such as UNIFAC.

COMPENTENCIES:
Accurate prediction of thermodynamic parameters for multicomponent systems

SERVICES

Predicting properties such as

- solubility
- partition coefficient (logP, logK_{OW})
- pK_a values
- activity coefficients, solvation energies, Henry constants, excess energies
- boiling points
- flash points

for applications such as:

- two- and three components phase diagrams (VLE/LLE) for distillation design
- prediction of vapour-liquid decompositions and solubility gap
- determination of optimal condition fluid-fluid extraction and solubility

TOOLS

- Gaussian software package
- AMS software package
- Dalton software package
- ORCA software

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