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Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

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The solubility of solid organic compounds in water and organic solvents is a fundamental thermodynamic property for many purposes such as product-process design and optimization, for the chemical and pharmaceutical industry. Experimental literature solubility data are usually scarce and temperature-dependent measurements are expensive in terms of time and resources. The few available data are badly organized and difficult to use for fast solubility calculations and solvent screening. Available models often require time consuming and complex implementation together with a good user expertise for their efficient use. In addition, most of the models are not predictive and requires experimental data for the calculation of the needed parameters.

This work aims at developing an efficient framework for the solubility modelling of Active Pharmaceutical Ingredients (API) in water and organic solvents. With this framework, the user will be able to solve a specific design/verification problem, quickly and simply with no expert knowledge. At first, a solubility database containing solid-liquid equilibrium data is developed. Then, available and validated models for the calculation of solid-liquid equilibrium (NRTL-SAC, PC-SAFT) are used for solubility calculations when the needed interaction parameters or experimental data are available. The CI-UNIFAC is instead used when the previous models lack interaction parameters or when solubility data are not available. A new GC^+ model for APIs solvent selection based on the hydrophobicity, hydrophilicity and polarity information of the API and solvent is also developed, for performing fast solvent selection and screening. Eventually, all the previous developments are integrated in a framework for their efficient and integrated use.

Two case studies are presented: the first highlights the solubility modelling tool for the calculation of APIs solubility in lipids with the PC-SAFT equation of state; the second highlights the solvent selection tool for the identification of feasible solvents for nitro-APIs.