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Solventpro: The Solvent Selection and Design Framework

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Solventpro – the Solvent Selection and Design Framework

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Solvents are widely used in a number of applications, for example, as separation agents, reaction mediums, cleaning agents and product carriers. The use of solvents may be classified as either required for processing (separation, reaction, cleaning) and/or as part of a chemical-based product (cosmetic products, delivery devices). While there are some solvent selection databases and special software for very specific applications, a comprehensive database and/or framework for the general solvent selection/design problem is lacking. Also, in many instances, solvents are selected from a list mainly by experience (previous experience or expert knowledge) and/or experiment based trial and error. Therefore, a systematic generic approach to solvent selection and design for all types of solvent use is highly desirable, even though it provides some challenges in terms of database management, inclusion of expert knowledge, model-based solvent design and integration of the various methods and tools within a generic framework. Such a systematic approach should ideally be model/data-based, encouraging innovation, and focused on experiment-based verification only as the last step before solvent application. An important additional aspect in solvent selection and design is the consideration of environmental impact, which is a crucial factor in the disposal (or waste) of industrial solvents. That is, the solvent selection and design framework must also incorporate the "Green Chemistry Principles".

In this paper, the computer-aided solvent selection and design framework, a comprehensive approach to solvent selection problem, called SolventPro, will be presented. The framework integrates different methods and tools needed to manage the complexity and solve a wide range of solvent related problems in an efficient, flexible and robust manner. In particular, new models for solubility predictions, multi-level property estimation as well as molecular and solvent blend design, solvents database, and, solution of interesting problems from industry will be highlighted. In particular, application of SolventPro to design and analysis of various solvent-based extraction processes will be illustrated.

An important feature to highlight of the SolventPro software is the development of problem specific templates for various solvent related problems such as, solvents for organic synthesis (including complex reaction systems), solvent-based separations (separations involving vapour-liquid, liquid-liquid and/or solid-liquid equilibrium systems), solvents for phase transfer catalysis (PTC) reactions, solvents for pharmaceutical industry (API solubility), solvents in formulations (as part of cosmetic and other solvent based formulations), and as cleaning agents. The goal of the template is to guide the average user through the essential and desirable steps in solvent selection and design. The expert may also use the general interface and create their own template for the types of solvent related problems they usually solve. The solvents database currently contains information about more than 1000 organic solvents and their properties, including environmental and transportation properties, and, there are about 1000 ionic liquids (IL), which may also be studied as potential solvents for extraction-based separation processes. There is an efficient search engine to find the solvents (organic or IL) and a corresponding method for computer aided molecular-mixture design. Property models library include state of the art group contribution[plus]based models for pure component as well as mixture property predictions. These predictive models allow the selection and/or design of innovative solvent based processes and/or products. Another feature of the model library is models used for solvent performance analysis/verification. For example, driving force diagrams for solvent-based separations; saturation diagrams for solid solubility; controlled release predictions for product delivery; and many more.

The SolventPro software has been developed using the Net Framework and Visual C++6 programming tool/language. It is based on plug-in architecture which means that it possible to extend the framework by adding new modules without changing source code or the architecture of the framework. SolventPro has been tested on different types of solvent related problems in the area of process-product design. In this way, the SolventPro software belongs to the F3 category, that is, Fast, Flexible and Future.

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