Computer-Aided Solvent Selection Framework

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COMPUTER-AIDED SOLVENT SELECTION FRAMEWORK

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Abstract: Organic solvents have of great importance in modern industry. They are widely used as a reaction medium, as a reactant or as carrier in chemical, fine chemical, pharmaceutical, food, and drugs industry. Also solvents are playing important role in separation processes, organic synthesis, product delivery and etc. [1]. Solvent selection/design is a complex process, which includes some levels for indentifying best candidates depending on different criteria for evaluating solvent performance.

However because of the excessive consumption and utilization in a wide range of industries, millions of tons solvents have to be disposed off every year [2]. Therefore, it becomes very important to minimize and optimize the use of organic solvents as much as possible, to achieve Green Chemistry Principles [3]. To this end, a systematic methodology to select greener solvent for the promotion of organic reactions (Figure 1) has already been developed [4,5]. This methodology is based on thermodynamic properties of solvents, reactants and products together with the knowledge of reaction chemistry and conditions. The current framework is a combination of knowledge from industrial practice and computer-aided tools for property prediction and computer-aided molecular design (CAMD) principles.

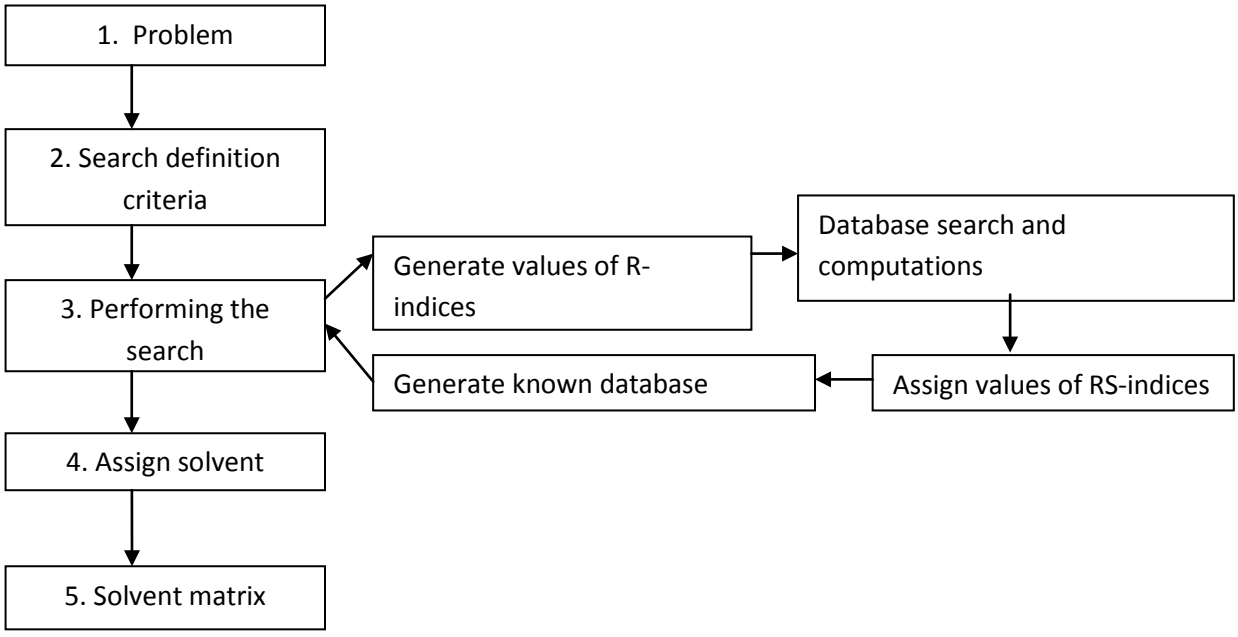

Figure 1. *A systematic rule-based methodology to identify a suitable solvent for organic synthesis*

Accordingly, the solvent selection occurs in two stages. In the first stage, a list of commonly used solvents is used to identify those solvents that match a sub-set of user-specified constraints, and based on this, a score allocated to each solvent. Simultaneously, a computer-aided molecular design (CAMD) technique is used to generate a list of solvents candidates which are ranked with

respect to their allocated scores. The scores are assigned from the calculated values of reaction-solvent (RS) indices following the reaction-solvent rules.

In the second stage, the candidate solvents are further evaluated through detailed calculations to identify most promising solvents for further experiments or other verification tests [6].

The Solvent Selection Framework is currently being extended to include multi-stage reactions, more complex reaction systems and other problems involving solvent substitution/selection in various types of solvent-based separations and cleaning.

References

1. R. Gani, C. J. Gonzalez, A. Kate, P. A. Crafts, A Modern Approach to Solvent Selection. Chemical Engineering Journal (2006), 30-43.
2. P. K. W. Lau, A. Koenig, Management, disposal and recycling of waste industrial organic solvents in Hong Kong. Chemosphere (2001), 44(1), 9-15
3. P.T. Anastas, J.C. Warner, Green Chemistry: theory and practice, Oxford: Oxford University Press, U.K., 1998
4. R. Gani, C .Jimenez-Gonzalez, D.J.C. Constable, Method for Selection of solvents for promotion of organic reactions. Computers and Chemical Engineering 29 (2005) 1661-1676.
5. M. Folic, R. Gani, C. Jiménez-González, D.J.C. Constable, Systematic Selection of Green Solvents for Organic Reaction Systems. Chinese Journal of Chemical Engineering. 16(3) (2008) 376-383.
6. M. Folic, R. Gani, C. Jiménez-González, D.J.C. Constable, P. Arenas Gomez, Solvents in Organic Synthesis: Replacement and Multi-step Reaction Systems. Computers and Chemical Engineering, 32(2008)2420-2444.