Simultaneous Process and Molecular Design through Property Integration

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Solvent selection has always been considered as one of the major tasks in process design. It entails finding the best solvents for a particular process that maximize its overall efficiency. In assessing the performance of a solvent, one should not only rely on its chemical constituency, but rather on the solvent's characteristics and effectiveness for the particular system, namely its properties, such as equilibrium distribution coefficient, critical point, volatility, solubility, density, etc.. Since these properties form the basis of the performance of many units, they can be primarily considered in order to select solvents, design and optimize a process system. For example, the performance of distillation depends on relative volatility, whereas extraction performance depends on the solubility of liquid solvents.

In this regard, property estimation plays an important role in characterizing the solvent utility for a certain process, and needs to be primarily evaluated at the design stage to yield feasible and optimum solvent candidates. So far, the selection of solvents has been typically carried out through screening of commonly used and already known solvents for particular applications. However, this could hinder the identification of new molecular structures and/or solvent blends that could achieve a better performance of the system. Therefore, solvent selection needs to be considered as a task of selecting a set of properties to target process performance, and has to be addressed simultaneously through synthesis at the molecular and process level. Moreover, molecular and process constraints need to be taken into account simultaneously, and process objectives need to be met. Obviously, if these constraints can be expressed through key-properties instead of key-compounds, this would provide a better understanding of the process and help addressing the solvent selection and process design problem more efficiently.

This paper presents a new graphical approach for solvent selection using property-based integration. It aims at providing a general framework for simultaneously representing molecular- and process- level property requirements based on which the system can be designed. The clustering concept is used to map the problem from the non-conserved property domain into the componentless cluster domain, whereas group contribution methods (GCM) are employed to estimate the properties of pure organic compounds based on structural groups. Property clusters are used to represent both molecular groups and process requirements on a ternary cluster diagram. Strategies for optimizing solvent selection based on cost and performance criteria are provided.

This work offers a starting point for considering new methodological approaches (including graphical, algebraic and mathematical programming techniques) for designing and optimizing property-oriented processes based on molecular information and process objectives. Finally, a case study is presented to illustrate the validity of the described approach.