Integrated Synthesis of Optimal Processes and Molecules for Solvent-Based Systems

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The work reports on a framework for the integrated design of processes and solvents. The approach relies on structural optimization and allows the identification of solvent molecules that achieve optimal process performance at low computational requirements. Current computer aided solvent design methods lack process performance feedback at the solvent design stage. As a result, solvents and processes are synthesized sequentially rather than interactively and current approaches are thus limited in their ability to identify good solutions to the overall design problem. These limitations are a result of the size and complexity of the design problem and the need for problem decomposition. Very few attempts have been made to systematically engage process synthesis and solvent design in a unified framework. We propose such a framework which allows the bilateral interaction and optimization between the two stages, is free of potentially biasing assumptions and capable of providing confidence in the optimal results.

In the proposed unified framework solvent, molecules are synthesized using computer-aided molecular design techniques based on multi-objective stochastic optimization. As a result, unnecessarily premature assumptions about the process requirements become redundant as each design objective is treated independently, freed of artificial constraints. While the interactions among a variety of objectives are thoroughly explored, the optimal search identifies a comprehensive set of solvents that represents molecules with a broad range of structural, physical and economic characteristics. One of these solutions will be the optimal solvent for a system with given process economics and constraints. This solvent will be identified in multiple process synthesis experiments. The introduction of the existing solvent molecules into process synthesis frameworks capitalizes on the available design information through the identification of molecular clusters, thus partitioning the molecular set into smaller compact groups of similar molecules. The paper will discuss different clustering strategies. A representative molecule from each identified cluster is introduced into the

process synthesis model as a discrete option and the result represents the economic impact of the solvent in the specific process. The obtained process cost for the representative molecule is then linked to the contents of the cluster through a probability distribution function that allows the stochastic comparison of solvent/process costs in various clusters without requiring process performance data for all the molecules. We therefore reveal the molecules that benefit process synthesis only by optimizing the process models for a few molecules.

Our implementation of the proposed framework employs proven process synthesis models for liquid-liquid extraction, gas-liquid absorption and reactive separation. For instance, the utilized reactive separation process synthesis models are represented by superstructures of generic reactor/mass exchanger units able to capture all possible novel and conventional design options that may exist for such systems (Linke and Kokossis, 2003, AIChE J., 1451).

The proposed methodology is illustrated with numerous industrial and academic case studies. When applied to examples from the literature, the obtained results compare favorably with results previously reported.