**243r Combining Group Contribution and Property Clustering Techniques for Visual Solution of Process and Molecular Design Problems**

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The terms product synthesis and design designate problems involving identification and selection of compounds or mixtures that are capable of performing certain tasks or possess certain physical properties. Since the properties of the compound or mixture dictate whether or not the design is useful, the basis for solution approaches in this area should be based on the properties themselves. However, the performance requirements for the solvent are usually dictated by the process and thus the identification of the desired solvent properties should be driven by the desired process performance. Traditionally process design and molecular design have been treated as two separate problems, with little or no feedback between the two approaches. Each problem has been conveniently isolated or decoupled from the other. When considering conventional process design methodologies, the selected species are chosen from among a list of pre-defined candidate components, therefore, limiting performance to the listed components. On the other hand, with molecular design techniques, the desired target properties are required input to the solution algorithm. Once again these decisions are made ahead of design and are usually based on qualitative process knowledge and/or experience and thus possibly yield a sub-optimal design. Introduction of the property integration framework allows for representation of process and products from a properties perspective. Utilizing this methodology enables identification of the desired product properties by targeting the optimum process performance without committing to any components during the solution step. The identified property targets can then be used as inputs for solving a molecular design problem, which returns the corresponding components. In this work, we are combining property clustering techniques and group contribution methods (GCM) to facilitate simultaneous consideration of the property performance requirements as well as process and molecular constraints. For visualization purposes only three properties can be used to characterize the system, however algebraic and optimization based approaches can extend the application range to include more properties. Using this approach the process requirements along with the molecular fragments can be represented on a ternary cluster diagram. The basis for the property clustering technique is the use of property operators, which are tailored to exhibit linear mixing rules. The mixing rules will invariably be functionally different for molecular groups and process streams; however since they represent the same property, they can still be visualized on the same diagram. Once visualized it is possible to solve the process design problem by identifying the solvent properties corresponding to the desired process performance. On the ternary diagram the target solvent properties will be represented as either a single point or a region depending on whether the target properties are discrete or given as intervals. The structure and identity of candidate solvents are then identified by combining or “mixing” molecular fragments until the resulting properties match the targets. A significant result of the developed methodology is that for problems that can be satisfactorily described by just three properties, the process and molecular design problems are solved visually and simultaneously on a ternary diagram, irrespective of how many molecularly fragments are included in the search space, This contribution will highlight the principles of the methodology along with a solvent design case study.