SCHOOL OF CHEMICAL & BIOMOLECULAR ENGINEERING
SPRING 2010 SEMINAR SERIES
FEBRUARY 3

DR. MARIO RICHARD EDEN

Mary & John H. Sanders Associate Professor of Chemical Engineering
Department of Chemical Engineering
Auburn University

"Property Based Techniques for Process and Product Design"

Introduction of the property integration framework has allowed for representation of processes and products from a properties perspective. 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 are then used as inputs for solving a molecular design problem, which returns the corresponding components. Recently, novel property clustering techniques and proven group contribution methods have been combined to facilitate simultaneous consideration of the property performance requirements as well as process and molecular constraints. The clusters are obtained by mapping property relationships into a low dimensional domain allowing for visualization of the problem. For visualization purposes only three properties can be used to characterize the system, however algebraic and optimization based approaches have extended the application range to include more properties. Using this approach the process requirements along with the molecular building blocks can be represented on a ternary cluster diagram.

The property clustering technique uses 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 product properties corresponding to the desired process performance. On the ternary diagram the target product properties will be represented as either a single point or a region depending on whether the target properties are discrete values or given as ranges. The structure and identity of candidate molecules 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 adequately described by just three

properties, the process and molecular design problems are solved visually and simultaneously on a ternary diagram, irrespective of how many molecular fragments are included in the search space.

Mixture design is a Design of Experiments (DOE) tool used to determine the optimum combination of chemical constituents that deliver a desired response (or property) using a minimum number of experimental runs. While the approach is sufficient for most experimental designs, it suffers from combinatorial explosion when dealing with the multi-component mixtures found in e.g. pharmaceutical excipient design. The property clustering technique can be used to overcome this limitation by significantly reducing the complexity of the mixture design problem.

While most current techniques make use of group contribution methods (GCM) to design molecules, there are many properties which can not be estimated by GCM. Furthermore, not all possible atomic arrangements and structures can be represented in GCM. Hence, there is a need of an efficient methodology for the design of structured molecules. One such approach to structured product design is to combine property clustering with decomposition techniques. This approach first utilizes multivariate characterization techniques to describe a set of representative samples, and then uses decomposition techniques such as principal component analysis (PCA) and partial least squares on to latent surfaces (PLS), to find the underlying latent variable models that describe the molecule's properties. The orthogonal nature of these models allows for group-based interpretations and property predictions which can be utilized to design new molecules not found in the original set of molecules.

This contribution will highlight the methodologies of this novel unifying design framework through illustrative examples of property driven process and product design.