Modeling and Computational Challenges in the Optimization of Chemical Process Systems

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In this presentation we give an overview of challenges in the development of models and algorithms for the discrete and continuous optimization of a variety of applications in Process Systems Engineering, and that have been largely the result of collaborations with industry. We first provide a brief overview of deterministic models based on mixed-integer linear/nonlinear programming (MILP/MINLP) to highlight the progress that has been made. We illustrate the application of these techniques in the integration of production planning and inventory control, as well as in the design of reliable chemical processes. Next, we provide a brief review of global optimization for which the progress is illustrated with the synthesis of integrated water networks, with the design of centralized and distributed manufacturing for biomass, and with the design and planning of infrastructures for shale gas production that involve large scale nonconvex MINLP models. We also address the handling of uncertainty in optimization models through approaches that are based on robust optimization and stochastic programming. For the former, we consider affine-adjustable recourse to avoid overly conservative results, and illustrate its application in cryogenic storage in air separation plants that participate in the electricity and operating reserve markets. For the case of stochastic programming, we consider first the development of strategies based on decomposition and that can handle a very large number of scenario; this we illustrate with optimal design of supply chains that are subjected to disruptions in their distribution centers. Finally, we consider multistage stochastic programming models that involve exogenous and endogenous parameters for which effective theoretical and solution methods are proposed. These are applied to the design and planning of offshore facilities with uncertain crude oil prices and reservoir sizes.