A Simulation-Based Superstructure Optimization Approach for Process Synthesis and Design Under Uncertainty

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Systematic frameworks to chemical and biochemical process design have been traditionally focused on mathematical programming-based approaches in which a deterministic superstructure optimization problem is formulated and solved using mixed integer nonlinear solvers (MINLP) to find an optimal design of a processing network. Although significant progress has been achieved in development of these MINLP solvers, wider application of these approaches is hindered by 2 major limitations: (1) the strict requirement of algebraic (mathematically trackable) modeling of the underlying processes, (2) the lack of consideration concerning the effects of uncertainties on the solution returned by deterministic optimization solvers. Therefore, there has been a significant interest in approaches bringing together the power of well-established understanding of process simulation technologies into the optimization-based process design frameworks which can also systematically integrate the available uncertainty information during its optimal design selection steps.

In recent years, simulation-based optimization emerged as a promising alternative to traditional mathematical optimization as it allows for detailed optimization of processes solely by making use of the input-output data of arbitrarily complex process simulations, without needing to make any optimization inference from the internal model structure (such as information of derivatives, etc.). In this work, we present a novel framework for process synthesis and design by combining the power of rigorous process simulation, advanced machine learning algorithms for optimization, and Monte Carlo simulations for design under uncertainty. The framework is implemented into a decision support tool, sustainable process synthesis and design (SPDLab), which uses an in-house Stochastic Kriging-based optimization solver to direct the search for the optimal design. The capabilities of the tool are demonstrated with a case study of selecting an optimal process design for an industrially-relevant scale wastewater treatment plant (WWTP) based on techno-economic performance metrics (effluent quality index (EQI) and operational cost index (OCI)), in which significant design variables are identified with a computationally efficient global sensitivity analysis using Gaussian process modeling with the Sobol sensitivity method. Furthermore, the effects of system uncertainties, such as variations in influent wastewater pollutant load and composition, cost of electricity used for aeration, and the price of biogas produced in sludge digesters, are incorporated into the stochastic estimation of the objective and technical performance constraint values (i.e. regulated effluent discharge limits) via a Monte Carlo simulations framework. Results obtained highlight the importance of considering the uncertainties at the early stage of design and show that the tool can provide significant insights into engineering design decision-making processes by incorporating all the available process understanding with the state-of-the-art process systems engineering methodologies.

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