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Towards Development of a Computational Framework for Sustainable Process Synthesis and Design

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The design of modern engineering systems has to comply with more and more stringent regulations, which are being introduced to meet today's sustainable development goals. Process systems engineering promotes the application of systematic computer-based methods to process design and synthesis, which encompasses a vast range of industries and requires integration of significant amount of knowledge from diverse scientific disciplines, practical industrial experience, and a number of tools and methods to carry out sustainable process design. One of the critical pain points faced by process design engineers is the lack of available tools regarding the comparative analysis and synthesis of alternative processing networks, which hinders the implementation of innovative processing configurations using newly arising process technologies. Given the lack of data regarding these new processes and the uncertainty in the available process data, there exists a need for new supporting methods and tools for both generating alternative processing flowsheets and assisting decision-makers with the selection of the optimum flowsheet under system´s uncertainties.

A new decision support tool named Sustainable Process Design Lab (SPDLab) is developed to address above-mentioned needs of design professionals. For that purpose, a new Monte Carlo-based process synthesis and design framework was developed and implemented in SPDLab. At the first step of the novel three-step-framework, a superstructure consisting of alternative treatment technologies is generated to represent alternative plant networks using factorial combination along with expert knowledge. A number of promising plant layouts are identified using highly parallelized exhaustive Monte Carlo simulations using the tool's extensive capabilities to align with the high-performance computing environments. In the final step, which uses an in-house stochastic-Kriging-based constrained derivative-free optimizer, the tool performs a simulation-based design optimization to further improve the selected designs and investigate their robustness against system uncertainties. The application of the tool is highlighted for process synthesis and design challenge in resource recovery from wastewater treatment plants (WWTPs).