A SIMULATION-BASED OPTIMIZATION APPROACH FOR PROCESS SYNTHESIS AND DESIGN OF WASTEWATER TREATMENT PLANTS

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Abstract

A paradigm shift is currently underway in the wastewater sector from considering wastewater as a waste to be treated to a valuable source that has an increased potential for energy production and resource recovery. New systematic model-based methodologies are needed to comply not only with the changing design objectives of the industry, but also with the increasingly stringent effluent quality regulations. In this work, we develop a novel simulation-based optimization framework for process synthesis and design of complex engineering systems whose accurate modeling requires a full-scale simulation, such as wastewater treatment plants (WWTPs). At the first step of the proposed three-step-framework, we postulate a superstructure comprising of alternative treatment technologies (including also the newly arising innovative technologies) and generate alternative plant networks using factorial combination along with expert knowledge. The second step identifies promising plant networks with the use of exhaustive Monte Carlo simulations, which are highly parallelized to align with the high-performance computing environments. The final step of the novel framework employs a model-based constrained derivative-free method to optimize the energy production of the plant using stochastic Kriging metamodels whose heteroscedastic variance information is used to represent inherent system uncertainties that are propagated with Monte Carlo simulations. The framework is applied to a case study of designing an energy surplus WWTP and the results show a potential for an increase in the energy production by about 20% compared to designs obtained from the second step without compromising the effluent quality.

Keywords

Simulation optimization, derivative-free optimization, Monte Carlo simulations, WWTPs

Introduction

Like many other engineering systems, wastewater treatment plants (WWTP) of today has grown quite complex, incorporating various physical, chemical, and biological processes under large system uncertainties to meet technical, economic, and regulatory performance requirements. Given a steadily growing number of competing treatment technologies and the ever-ambitious performance goals, the need for the use of simulation, optimization, and systematic process synthesis methodologies for engineering design of WWTPs is becoming more pronounced among design professionals. A realistic modeling of such complex systems requires the use of first principle simulation models in the form of systems of nonlinear ordinary/partial differential equations to account for the spatial and temporal variation of the system properties. As the algebraic models are often inadequate to allow for detailed representation of such systems, the traditional mathematical programming techniques, such as

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MINLP literature, cannot be readily used for the process synthesis and design problems arising in those systems. Derivative-free optimization (DFO) literature, however, offers a promising alternative for the optimization of such systems, as they do not require derivative information to locate a global optimum, hence the name, using only the simulation input-output data to optimize a black-box system.

In recent years, research on applications of derivative-free optimization algorithms in process systems engineering frameworks has flourished (Bajaj et al., 2018; Wang and Ierapetritou, 2018; Beykal et al., 2018). As WWTP systems are subject to large systems uncertainties, i.e. variations in influent loadings, model uncertainties, etc, with requirements to meet effluent quality limits, we turn our attention to the stochastically constrained DFO algorithms with surrogate model-based search methods. One increasingly popular example of such algorithms is stochastic Kriging (Ankenman et al., 2010), which uses a stochastic process model to characterize a system with heteroscedastic noise variances. Unlike other surrogate models, it accounts for variance information of simulation outputs during its construction, which makes it more suitable for modeling stochastic systems like WWTPs. In this paper, we propose a new process synthesis and design framework for WWTPs. The two main methodological contributions of the paper are a Monte Carlo simulation based superstructure optimization approach for process synthesis and a constrained derivative-free optimization (CDFO) framework using stochastic Kriging models with Monte Carlo simulations for process design optimization under uncertainty. The details of the generic framework is outlined in the following.

The Framework

The overall scheme of the proposed framework is shown in Figure 1. The framework addresses the goal of finding promising networks for a given design objective (step 1 and 2) and the goal of optimizing a given network separately (step 3).

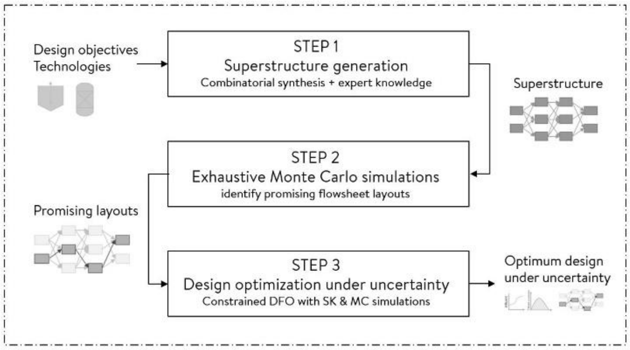

Figure 1: Schematic of the proposed framework

Table 1 gives more detailed steps of the constrained DFO algorithm of the framework, which uses a stochastic infill criterion, expected quantile improvement (EQI) (Picheny and Ginsbourger, 2014), to return a new sampling design point to perform plant-wide simulations.

Table 1. The constrained DFO algorithm with stochastic Kriging (SK) and Monte Carlo simulations

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Algorithm  Constrained DFO with SK and MCS
STEP 1.1: Create an input space of decisions variables and sample using a space filling design. (LHS, Sobol, etc.)
STEP 1.2: Perform WWTP simulations to create a DOE
STEP 1.3: For each design point in the DOE, perform MC simulations to propagate the influent uncertainty.
STEP 1.4: Construct stochastic Kriging models of the objective and the constraints using the DOE and MCS.
STEP 2: while $(n < N_{max})$
    Step 2.1   Find the next candidate point $x_{n+1}$ by optimizing an infill criterion. (EQI)
    Step 2.2   Simulate the WWTP at $x_{n+1}$. Include the response in the initial DOE if it is a new response.
    Step 2.3   Update the SK models using the new DOE.
    Step 2.4   Update the current best point $x^*$.
Step 3:   Return the best solution found so far, $x^*_{Nmax}$
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Conclusions

This paper presented a novel generic framework, which allows synthesizing and optimizing new WWTP networks for a given objective while meeting technical performance requirements under the significant uncertainties inherent in innovative technologies, influent loadings, etc.

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