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Improving Speed and Efficiency of Global Sensitivity Analysis Using Metamodeling-Based Approach: A Case Study on Wastewater Treatment Plant Modeling

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Global sensitivity analysis (GSA) provides model developers with invaluable insights into the interactions between uncertain model parameters and model output uncertainty. Among its large class of applications are identifying relevant input variables for uncertainty quantification, model quality assessment, model selection, calibration, optimization, to name a few. In the wastewater treatment modelling community, several global sensitivity analysis techniques using Monte Carlo (MC) approach has been applied. (Sin et al., 2011; Cosenza et al., 2013; Ramin et al. 2014). Although the MC approach to sensitivity analysis is relatively well established, it requires a large number of model evaluations (typically in the order 10^4 for variance decomposition based techniques) to estimate sensitivity indices of each parameter accurately, making its use impractical for computationally intensive models such as wastewater treatment process models. In an alternative approach, the original model behavior is approximated using computationally less costly metamodels (also referred to as surrogate models), which are then used to calculate Sobolâ€™ sensitivity indices. Two of the most efficient type of metamodels used for this purpose are polynomial chaos expansions (PCE) (Sudret, 2008) and Gaussian process (GP) models (Marrel et al., 2009).

This study explores applications of these surrogate models for performing global sensitivity analysis of models used within the BSM2 framework. To this end, three different scenarios are framed. The first scenario looks into the case of uncertain influent fractionation (pollutant loads), the second into the uncertain stoichiometric and biokinetic parameters of Activated Sludge Model 1 (ASM1) whereas the third investigates sensitivity of secondary settler model to hydraulics and design related parameters. Experimental designs (i.e. learning sample) are generated using two different space-filling sampling algorithms, i.e., Latin hypercube sampling and Sobol sequence (quasi-Monte Carlo) and surrogate models of type PCA using least angle regression and GP model are constructed. Confidence intervals of the sensitivity indices are also estimated using the bootstrap method for PCE and the internal model structure of GP. Sobol sensitivity indices of metamodeling-based approach showed great similarity with those obtained from MC approach for each of the investigated scenarios, yet with much faster computation times. An experimental design size of 200 was found to be adequate to construct efficient surrogate models. Effect of using different sampling algorithms was found negligible. Further, the obtained results also suggest surrogate models can efficiently be used to replace complex mechanistic models used in wastewater treatment for complex modelling needs.

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