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Monte Carlo based Sensitivity Analysis and Derivative-free Optimisation

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Global sensitivity analysis (GSA) and derivative-free optimisation (DFO) methods share a common task which is the multiple evaluation of black box models. For sensitivity analysis the value sets in the sample hypercube are evaluated and the output vector is stored to then post-process this input-output data relation with different GSA methods. In case of DFO, initial estimates of the variables are sent to the black box model and then the result is evaluated in respect to a stopping criterion. If the criterion isn't met then a new input set is defined and sent to the black box model, whereas the evaluation loop stops if the criterion is satisfied and an optimum is found. We developed a Python based COM-interface to the ProII process simulator to analyse several case studies. Sensitivity analysis methods were applied to a heat pump system [1] and a molecular distillation process [2] to retrieve sensitivity indices for the consumption of power (COP) or the beta-carotene recovery subject to critical temperature, critical pressure and acentric factor which the Soave-Redlich-Kwong equation of state depends on. Sobol sensitivity analysis and Morris screening were performed for both cases. A three-step glycerol purification process was optimised via DFO to obtain the optimal values for the operating parameters (T_{Unit}, P_{Unit}) and the feed flowrate to the system of three evaporation units. The optimizer RBFopt and surrogate modelling, namely polynomial chaos expansion, were applied to solve for the operating point close to the optimum. The results show that the Python-COM interface is a valuable tool to connect process models in a simulator with more advanced sensitivity and optimisation techniques.

[1] Frutiger, J., Zühlsdorf, B., Elmegaard, B., Abildskov, J., Sin, G., Reverse Engineering of Working Fluid Selection for Industrial Heat Pump based on Monte Carlo Sampling and Uncertainty Analysis, Industrial & Engineering Chemistry Research 57 (40) (2018) 13463-13477. doi: 10.1021/acs.iecr.7b04607
[2] Tehlah, N., Kaewpradit, P., Mujtaba, I. M., Development of Molecular Distillation based Simulation and Optimization of Refined Palm Oil Process based on Response Surface Methodology, Processes 5 (3) (2018). doi: 10.3390/pr5030040