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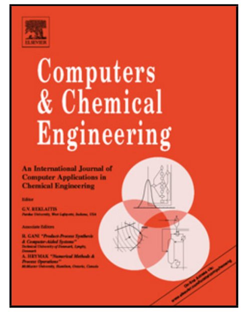

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Probabilistic reactor design in the framework of elementary process functions

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Abstract

Computational process models in combination with innovative design methodologies provide a powerful reactor design platform. Yet, model-based design is mostly done in a pure deterministic way. Possible uncertainties of the underlying model parameters, prediction errors due to simplifying assumptions regarding the reactor behavior and suboptimal realizations of the design along the reaction coordinate are in general not considered. Here we propose a systematic design approach to directly account for the impact of such variabilities during the design procedure. The three level design approach of Peschel et al. (2010) based on the concept of elementary process functions (EPF) serves as basis. The dynamic optimizations on each level are extended within a probabilistic framework to account for different sources of randomness. The impact of these sources on the performance prediction of a design is quantified and used to robustify the reactor design aiming at a more reliable performance and thus design prediction. The uncertainties of model parameters, non-idealities of the reactor behavior and inaccuracies in the design are included via statistical moments. By means of the sigma point method (Julier and Uhlmann, 1996) random variables are mapped to the design objective space via the nonlinear process model. Importantly, this work introduces a full probabilistic orthogonal collocation approach, i.e. random and stochastic variables can be described. Whereas the former one relates to randomness independent on the reaction time (e.g. kinetic model parameters or initial conditions), the latter one describes stochasticity along the reaction time (e.g. fluctuating pressure or temperature control). As an example process the hydroformylation of 1-dodecene in a thermomorphic solvent system consisting of n-decane and N,N-dimethylformamide is considered.

Our probabilistic EPF approach allows designing robust optimal reactors, which operate within an estimated confidence at their expected optimum considering almost any kind of randomness arising in the design procedure. An additional value is that with increased predictive power of the reactor performance its embedding in an overall process is strongly simplified.

Keywords:

Hydroformylation, Multiphase systems, Probabilistic reactor design, Robust design optimization, Optimization under uncertainty