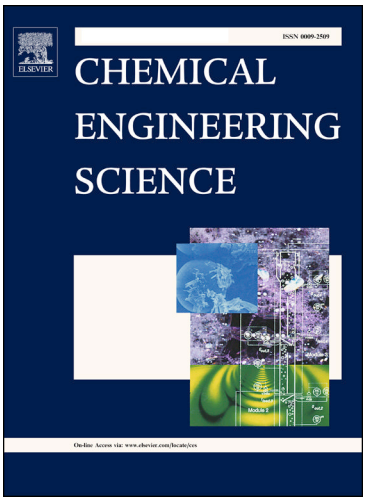

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Optimization Under Uncertainty in Chemical Engineering: Comparative Evaluation of Unscented Transformation Methods and Cubature Rules

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Abstract

Model-based optimization under consideration of uncertainty is an important and active research topic. In order to handle uncertain model and process parameters for the design and optimization of chemical processes, various different approaches have been proposed in the literature. Among these approaches, the application of unscented transformation (UT) methods received increasing attention recently. The UT is used to calculate approximations of the first two statistical moments of the objective and constraints which are implemented in the formulation of the optimization problem. Since the UT only allows for approximations of the statistical moments, the approximation error inevitably influences the optimization. In the present contribution, we emphasize that a poor approximation significantly reduces the meaningfulness of an optimization under uncertainty approach. Hence, we compare a variety of UT methods and study the effect of their corresponding tuning parameters on the approximation accuracy. Furthermore, we investigate four different cubature rules which are well known from the numerical integration literature and which show similarities to the UT from an implementational point of view.

The individual methods are compared in terms of approximation accuracy and computational effort based on examples from chemical reaction engineering. Our results indicate that the cubature rule labeled as CU51 provides the most accurate results at reasonable computational costs. The recently proposed cubature rule labeled as MSSRC provides less accurate results, but is computationally more efficient than the CU51 rule and is thus an attractive alternative. Regarding the UT methods, the results show that the proper choice of the tuning parameter