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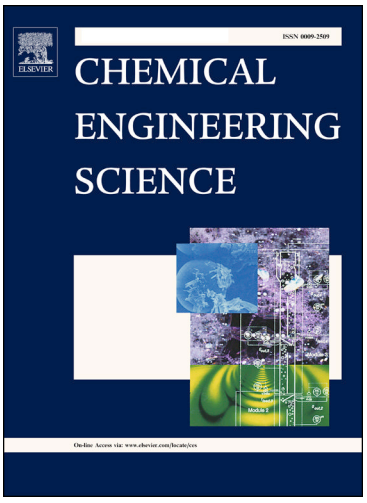

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Parameters Estimation and Model Discrimination for Solid-Liquid Reactions in Batch Processes

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Abstract

Process optimization and control rely highly on system modeling. A reliable model must be formulated with estimable parameters in order to closely predict system behavior in the operating domain. This paper focuses on the modeling and parameter estimation of organic solid-liquid reactions in batch reactors with limited lab-scale experimental data and industrial-scale plant data. Two possible mechanisms, shrinking particle model and dissolution model, are reviewed. A uniform dynamic model with a model indicating factor and several lumped parameters is developed for both mechanisms. A Bayesian estimation procedure is discussed and implemented to select an estimable parameter set, simplify the system model, obtain prior information and determine posterior parameter values. The quality of estimation results is analyzed and enhanced by examining the parameter covariance matrix at the optimal point. In the case of multiple candidate process models, model discrimination is then performed to choose the best representative one by comparing posterior probability shares. Finally, the selected model is validated and tested.

Keywords: Solid-liquid reactions, Dynamic modeling, Bayesian estimation, Model discrimination

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