A Single Platform Approach For Kinetics Identification, Reaction Engineering, And Model Deployment

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Abstract

Chemical reaction kinetics identification is an essential and enabling step for reaction engineering designs. This presentation explores the COMSOL platform for performing the kinetics estimation and subsequent reaction engineering of a catalytic reaction with formation of competing products. Seeking the dependencies of the reaction kinetics on the catalyst concentration and reaction temperature, COMSOL's ability to freely define parameters for identification enables one-step success in estimating all the parameters from the experimental data. In contrast, the existing tool(s) usually requires a two-step approach, separating the identification of catalyst dependency and temperature dependency. Furthermore, the identified chemical kinetics is conveniently extended to a reaction engineering study in COMSOL, where design specs of a plug-flow reactor are generated for conversion and selectivity. Empowered by the COMSOL application builder and server, the model is deployed to users with easy accessibility for running simulations on demand.