A Dynamic Simulation of Heterogeneous Catalysis with COMSOL Multiphysics® Software

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Abstract

In this work, dynamic simulation at particle scale using COMSOL Multiphysics® software is carried out to predict the kinetics of solid catalyzed esterification reaction between acetic acid and methanol to produce methyl acetate and water. The reaction kinetic data utilized for modeling and validation is from the esterification reaction with solid catalyst such as Indion 180. It was observed that the reaction rate and kinetics inside the pores of the catalyst is of higher magnitude as compared to bulk of the liquid. When the reactant mixture is mixed with solid catalyst particles it becomes a uniform particulate-liquid suspension at sufficiently high mixing speed in a batch reactor. Keeping this as hypothesis for the determination of kinetics where each solid catalyst particle is surrounded by reactant mixture which is of equal volume for all the catalyst particles, a dynamic simulation is carried out using COMSOL Multiphysics® software which has solver for diffusion-reaction equation for both in liquid phase and inside particle. The intrinsic reaction rate constants for bulk liquid phase and inside the particle are obtained by solving the full diffusion-reaction equation and optimization method. Three different models are proposed for evaluating the rate constants from the experimental kinetic data. One of the model shows very good agreement with the experimental data.
Key words: Diffusion; Reaction; Esterification; Kinetics; Simulation; Catalysis

Figures used in the abstract

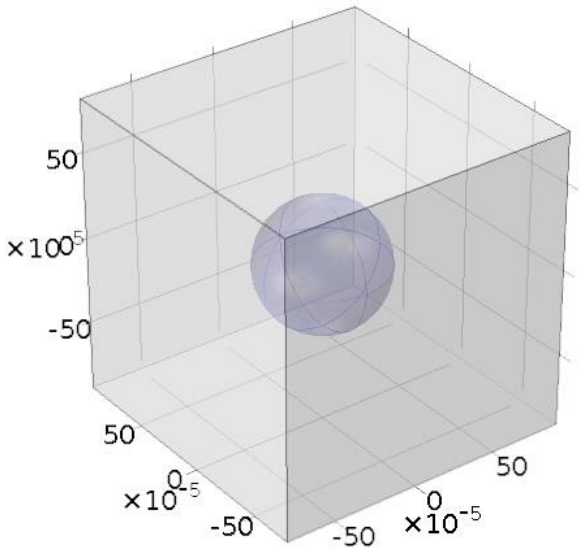

Figure 1: Geometry in simulation built with COMSOL Multiphysics® software for the catalyst particle surrounded by a cube of reactant liquid mixture. Units of length is in meters.

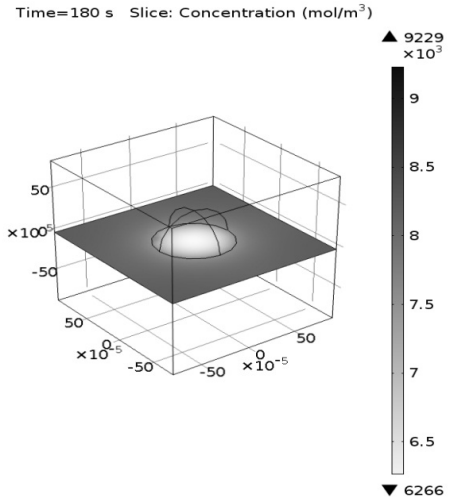

Figure 2: Spatial concentration distribution inside the catalyst particle and around it in the solution at an instant of time during dynamic simulation.