EXPLORATION OF MAXWELL-STEFANS PARTICLE DIFFUSION IN A KINETIC MODEL FOR BISPHENOL-A SYNTHESIS CATALYZED BY STRONG ACID CATION EXCHANGE RESINS

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Abstract

This work explores the use of a detailed Maxwell-Stefan diffusion model vs. a simplified Fickian diffusion model for a multi-component system, which was applied to the Bisphenol-A synthesis catalyzed by strong-acid cation exchange resins.

Keywords

Particle Diffusion, coupled reactor-particle model, Maxwell-Stefan diffusion

Introduction

The focus of this work is to compare two commonly used diffusion models for multi-component systems. The simpler Fickian diffusion model is compared with the Maxwell-Stefan model for a liquid reactive system. The reactive chemistry used as an example is the synthesis of bisphenol-A (BPA) which is an important chemical employed to make polycarbonate plastics and epoxy resins. Bisphenol-A (BPA) is synthesized by the condensation of acetone with two equivalents of phenol. A strong acid ion exchange resin can catalyze the reaction as seen by Yadav and Kirthivasan, (1997) and Reineker and Gates (1974).

This study uses a Langmuir-Hinshelwood mechanism to describe the reaction mechanism. The batch reactor was coupled with reaction and diffusion in porous particle model to estimate reaction rates and adsorption coefficients. Both models were used to fit kinetic rate parameters to experimental data. The two models were then used to explore the regimes where the results are almost identical and where the two models diverge in their respective predictions.

Model Equations

The concentration profile of each component in a representative catalyst particle yields the component fluxes at the external surface of the catalyst. The equation of continuity for a single component in a spherical particle with radial diffusion is given as:

$$0 = -\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 j_{i,r}\right) + S_i$$

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where r is the radial coordinate, $j_{i,r}$ is the molar flux of component i, S_i is the source term. The equation is solved assuming pseudo-steady state and negligible convective flow inside the porous particle. The flux was solved using two different models below as suggested by Solsvik and Jakobsen (2011):

(a) Fickian diffusion: $j_i = -cD\nabla x_i$

(b) Maxwell-Stefan diffusion: $$j_i = \frac{-c\nabla x_i + \sum_{j=1, j\neq i}^{n} \frac{j_j x_i}{D_{ij}}}{\sum_{j=1, j\neq i}^{n} \frac{x_j}{D_{ij}}}$$

Where x_i is the mole fraction, D is the average diffusivity, and c is the average molar density.

Conclusions

Results will be compared by fitting experimental data with the two diffusion models. We would like to present the conditions where the simpler Fickian model is applicable and can be used and where the more computationally-demanding Maxwell-Stefan equations are needed. The differences in the predictions with the two models will also be presented. Representative results (Figure 1) that show that Maxwell-Stefan equations predict that bigger particles will have an increased selectivity towards undesirable impurities as compared to the simpler Fickian model predictions. The very different diffusivities of individual species can be accounted with Maxwell-Stefan equations and leads to this result.

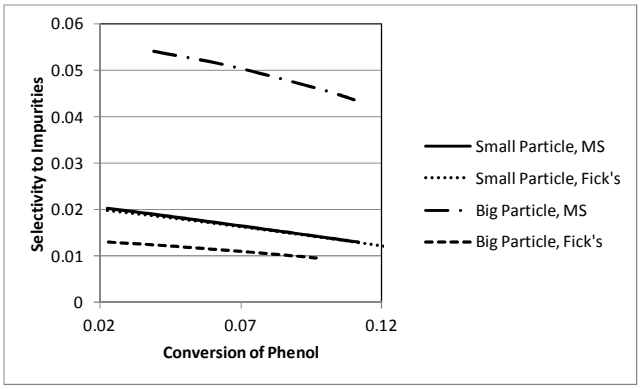

Figure 1. Effect of diffusion model on prediction of impurities formed in bisphenol-A production

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