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Prediction of effective reaction rates in catalytic systems of multiple reactions using one-dimensional models

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Abstract. In this work two one-dimensional (1D) models are used to approximate the catalytic behavior of three-dimensional (3D) shaped pellets. One of the 1D models employs a single parameter and is identified as Generalized Cylinder (1D-GC), while the second model, named Variable Diffusivity model (1D-VD), makes use of three parameters. Both models have been introduced in previous contributions and their performances were successfully tested for single catalytic reactions. A conventional system of two first order reactions in series and the process of selective hydrogenation of butadiene in the presence of 1-butene that shows strong inhibition effects are considered. The pellet shapes for which the largest errors were detected when using the 1D models in the cases of a single reaction were selected for this study. It was found that the use of the 1D-GC model leads to errors in the estimation of the effective reaction rate of up to around 7% for the first-order series-reaction system and up to 20% for the hydrogenation selective process. In contrast, the 1D-VD model can be used with a maximum error of the order of 1% for the first-order series-reaction system and about 4% for the selective hydrogenation system.

Key words: effective reaction rates, 1D models, reaction-diffusion, multiple reaction systems.

1. Introduction

The reaction –diffusion equations inside non-spherical catalytic pellets should be expressed in two (2D) or, in general, three (3D) spatial dimensions. An analytical solution will be possible only for linear kinetic and flux models and for isothermal conditions. It follows that most frequently a numerical solution will be needed for solving the conservation