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New numerical algorithm for solving multidimensional heterogeneous model of the fixed bed reactor

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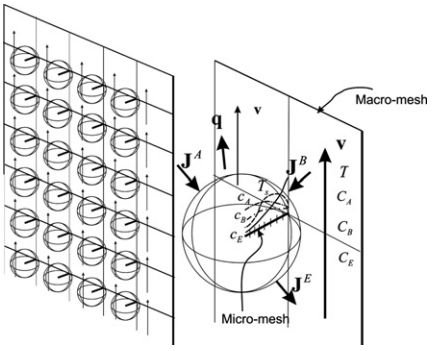
HIGHLIGHTS

- A new multiscale numerical model for simulation of a fixed bed reactor is proposed.
- The model uses two-level finite element mesh system.
- All important phenomena occurring in methanol synthesis were simulated.
- A mechanism of the hot spots (thermal runaway conditions) was modeled.

GRAPHICAL ABSTRACT

Two-level multidimensional modeling approach to simulation of a process in a fixed bed reactor.



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ABSTRACT

Although there are many approaches to modeling of fixed-bed reactors none of the heterogeneous models is thoroughly solved in the space of all the four dimensions: the axial and radial directions of the reactor, catalyst particle radius and time. The full heterogeneous model of the fixed-bed reactor has been proposed and a new algorithm for numerical solution of the mathematical model developed in this paper. As a practical case study the proposed method is applied to simulate methanol synthesis fixed-bed reactor working under industrial conditions. The proposed algorithm of solving the set of differential equation for the momentum, mass and energy balances for the heterogeneous model proved to be very effective thanks to a universal coupling of macro- and micro-geometries represented by two finite element meshes system. The solution of the multidimensional model of methanol synthesis in a fixed bed reactor allows to follow concentration and temperature profiles not only along the catalyst height but also in radial direction as well as inside porous catalyst particle. The application of the numerical solution of the multidimensional heterogeneous model of methanol synthesis in the fixed bed revealed interesting phenomena inside the catalyst and in the reactor. An occurrence of the temperature maximum in a middle axial position due to change of both reversible reactions of methanol synthesis and water gas shift reaction from forward to backward direction was observed. The evolution in time of hot spots (temperature propagation) due to local decrease of catalyst diameter and bed porosity was demonstrated by using a transient simulation of the process.

1. Introduction

One of the most commonly used type of chemical reactors in the chemical and petrochemical industry is the fixed bed reactor where the fluid phases flow through a packed beds of solid catalyst

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