



Numerical evaluation on the intraparticle transfer in butylene oxidative dehydrogenation fixed-bed reactor over ferrite catalysts



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ABSTRACT

Ferrite catalysts with high intraparticle pore volume and surface area are frequently used in the oxidative dehydrogenation of butylene. Whether the non-inclusion of intraparticle transfer limitation in fixed-bed reactors for oxidative dehydrogenation over ferrite catalysts in previous studies is appropriate remains unclear. In this study, we attempt to verify this process using a multi-scale modeling technology. The multi-scale model consists of a porous medium model and a single particle model under the oxidative dehydrogenation condition. This model can predict the influences of intraparticle transfer on the main component distributions in reactors and demonstrate that the intraparticle transfer limitation is obvious.

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Introduction

Intraparticle molecule diffusion and heat transfer should be involved in gas–solid multi-phase catalytic reactors because reactions occur at the active sites of catalyst particles [1]. A multi-scale structure (i.e., single catalyst particles, particle clusters/bubbles, and reactor scale) and multi-scale phenomenon (i.e., hydrodynamics, heat and mass transfer, and catalytic reaction kinetics) exist in this reaction process [2]. Therefore, these factors should be considered when gas–solid catalytic reaction occurs in a reactor.

The multi-scale phenomenon in reactors has recently attracted much attention [1], and various teams have developed multi-scale reactor models to describe the multi-scale phenomenon in gas–solid multi-phase catalytic reactors. Li et al. [3] developed the energy minimization multi-scale (EMMS) model for particle–fluid flow in gas–solid fluidized bed reactors (FBRs). The EMMS model was subsequently modified as an analytical multi-scale method to elucidate its principles [4–6]. Wang et al. [7,8] suggested a multi-scale CFD model to describe the gas–solid flows in FBRs for FCC. Yang et al. [9] constructed a multi-scale model that considered the heat transfer, mass transfer, momentum transfer, and fluid flow

with reactions at different spatiotemporal scales for the riser reactor of secondary reactions of fluid catalytic cracking gasoline. Dompazis et al. [10] developed a comprehensive multi-scale, multi-phase, and multi-compartment dynamic model to analyze the extent of particle segregation in the catalysis in gas-phase ethylene-propylene copolymerization FBRs. Andersson et al. [11] presented a multi-scale simulation method for modeling dispersions in a novel multiphase reactor, which is a continuous reactor that consists of repeated identical small mixing elements. Ghouse et al. [12] developed a multi-scale, dynamic, two-dimensional, and heterogeneous model for catalytic methane reforming. Chen et al. [13] developed a multi-scale CFD model based on a direct concurrent multi-scale approach. This technique incorporates a single particle model (SPM) and a two-phase CFD model to predict the effects of intraparticle transfer in the flow field and main composition distributions of a catalytic reaction that converts methanol to olefins in an FBR. Based on a similar approach, Zhu et al. [14] developed a multi-scale CFD model to describe the flow behavior and catalytic hydrogenation of dimethyl oxalate in an FBR. To model fixed-bed thermo-chemical processes of biomass as a multi-scale problem, Anca-Couce et al. [15] presented a multi-scale model considering the molecule, particle, and reactor levels. A framework for a multi-scale model for dynamic fixed-bed/moving-bed thermo-chemical conversion processes and the respective numerical solution method were introduced in their work. However, this model was not built based on the CFD

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Nomenclature

A_i	kinetic parameter of the i th step, $\text{mol} \cdot \text{kg}(\text{catalyst})^{-1} \cdot \text{h}^{-1} \cdot \text{Pa}^{-1}$
B	permeability factor
$C_{p_{cat}}$	mass heat capacity of catalyst, $\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
C_{p_i}	mass heat capacity of i component, $\text{kJ} \cdot \text{kg}^{-1} \cdot \text{K}^{-1}$
d_0	catalyst average diameter, m
$D_{i,eff}$	effective diffusion coefficient of the i th component, $\text{m}^2 \cdot \text{s}^{-1}$
D_{im}	Fick diffusion coefficient of the i th component, $\text{m}^2 \cdot \text{s}^{-1}$
D_{ik}	Knudsen diffusion coefficient of the i th component, $\text{m}^2 \cdot \text{s}^{-1}$
E_g	total fluid energy, $\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$
E_s	total solid medium energy, $\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$
f	Fanning coefficient
g	gravitational acceleration, $\text{m}^2 \cdot \text{s}^{-1}$
$h_{i,g}$	heat transfer coefficient, $\text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-1}$
H_i	enthalpy of the i th component, $\text{kJ} \cdot \text{kg}^{-1}$
h_i	species enthalpy of formation, $\text{kJ} \cdot \text{kg}^{-1}$
\bar{I}	identity matrix
$J_{i,r}$	mass diffusion flux, $\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$
\bar{J}_i	diffusion flux of species i , $\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$
$k_{i,g}$	mass transfer coefficient, $\text{m}^2 \cdot \text{s}^{-1}$
k_i	intrinsic rate constant of the i th step based on species mass fraction, $\text{mol} \cdot \text{kg}(\text{catalyst})^{-1} \cdot \text{h}^{-1} \cdot \text{Pa}^{-1}$
k_f	fluid phase thermal conductivity, $\text{W} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
k_s	solid medium thermal conductivity, $\text{W} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
k_{eff}	effective thermal conductivity of the medium, $\text{W} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
M	mixture fluid molar mass, $\text{kg} \cdot \text{kmol}^{-1}$
M_i	molar mass of the i th component, $\text{kg} \cdot \text{kmol}^{-1}$
M_0	mixture fluid molar mass at bulk, $\text{kg} \cdot \text{kmol}^{-1}$
N_r	number of chemical species
p	pressure, kPa
Pr	Prandtl number
Q_r	heat flux, $\text{J} \cdot \text{m}^{-2} \cdot \text{s}^{-1}$
r_0	catalyst particle radius, m
r_i	reaction rate of the i th step, $\text{mol} \cdot \text{kg}(\text{catalyst})^{-1} \cdot \text{h}^{-1}$
R	ideal gas constant, $\text{kJ} \cdot \text{kmol} \cdot \text{K}^{-1}$
Re	Reynolds number
Re_i	Reynolds number of the i th component
R_i	reaction rate, $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
Sh_i	Sherwood number of the i th component
S_c	Schmidt number
\bar{S}_i	mass source of the i th component of single model, $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
S	heat source of single model, $\text{J} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
s	surface conditions
\bar{S}	source term for the momentum equation, $\text{kg} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
Sh_f	fluid enthalpy source term, $\text{J} \cdot \text{m}^{-3} \cdot \text{s}^{-1}$
T	temperature, K
T^s	temperature at particle outer surface, K
u	apparent gas velocity, $\text{m} \cdot \text{s}^{-1}$
\vec{v}	gas velocity vector, $\text{m} \cdot \text{s}^{-1}$
\vec{v}^T	transpose of velocity vector, $\text{m} \cdot \text{s}^{-1}$

$v'_{i,r}$	stoichiometric coefficient for reactant i in the r th reaction
$v''_{i,r}$	stoichiometric coefficient for product i in the r th reaction
$\eta'_{i,r}$	rate exponent for reactant species j in the r th reaction
$\eta''_{i,r}$	rate exponent for product species j in the r th reaction
v_r^s	gas velocity at particle outer surface, $\text{m} \cdot \text{s}^{-1}$
Y_i	mass fraction of the i th component
Y_i^s	mass fraction of the i th component at the particle outer surface
$Y_{i,0}$	mass fraction of the i th component at bulk
ε	catalyst porosity
ρ_g	mixture gas density, $\text{kg} \cdot \text{m}^{-3}$
ρ_0	mixture fluid density at bulk, $\text{kg} \cdot \text{m}^{-3}$
ρ_{cat}	real catalyst density, $\text{kg} \cdot \text{m}^{-3}$
ρ_i	the i th component density, $\text{kg} \cdot \text{m}^{-3}$
μ	mixture fluid viscosity, $\text{Pa} \cdot \text{s}^{-1}$
$(\sum_v)_i$	diffusion volume of the i th component, $\text{cm}^3 \cdot \text{mol}^{-1}$
λ	thermal conductivity, $\text{W} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
λ_i	thermal conductivity coefficient of the i th component, $\text{W} \cdot \text{s}^{-1} \cdot \text{K}^{-1}$
η	effectiveness factor of the i th step
ϕ	medium porosity
τ	curvature factor
$\bar{\tau}$	shear stress of gas phase, Pa
Nu_i	Nusselt number of the i th component

approach. Most of the early multi-scale modeling efforts in this field are practically multi-scale gas–solid two-phase FBRs [16]. Furthermore, to the best knowledge of our knowledge, no open report has been published regarding the development of a multi-scale CFD model for catalytic fixed-bed reactors.

Considered a typical example of a multi-scale fixed-bed reactor, the fixed-bed reactor for the oxidative dehydrogenation of butylene to butadiene (ODOBTB) is very important in the chemical industry [17]. Ferrite catalysts with high intraparticle pore volume and surface area are frequently used in the ODOBTB [18]. However, the majority of previous studies on ODOBTB over ferrite catalysts have focused on the oxidative dehydrogenation mechanism and kinetics. Few studies have examined the oxidative dehydrogenation reactors, particularly the multi-scale flow and reaction phenomenon in these reactors, which can be used to evaluate more accurately the reactor performance. Xiang et al. [19] developed a mathematical model for the dehydrogenation of butylene into butadiene in an FBR. Elementary and secondary reactions were incorporated in their model. Borio et al. [20] established a dynamic mathematical model for the dehydrogenation of butylene to butadiene in a fixed-bed reactor, which was used to optimize reactor operation conditions and improve the butadiene production rate. However, the catalyst intraparticle transfer was ignored in their work.

In this study, a multi-scale model is applied to describe the impacts of intraparticle transfer on the flow field and main composition distributions in a fixed-bed reactor for the ODOBTB over ferrite catalysts. This model uses a porous medium model coupled with a spherical porous pellet model and reaction kinetic model. Based on the multi-scale model, this simulation study

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