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Simulation with a structure-based mass-transfer model for turbulent fluidized beds

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ABSTRACT

A structure-based mass-transfer model for turbulent fluidized beds (TFBs) was established according to mass conservation and the balance of mass transfer and reaction. Unlike the traditional method, which assumes a homogeneous structure, this model considered the presence of voids and particle clusters in TFBs and built correlations for each phase. The flow parameters were solved based on a previously proposed structure-based drag model. The catalytic combustion of methane at three temperatures and ozone decomposition at various gas velocities were used to validate the model. The TFB reactions comprised intrinsic reaction kinetics, internal diffusion, and external diffusion. The simulation results, which compared favorably with experimental data and were better than those based on the average method, demonstrated that methane was primarily consumed at the bottom of the bed and the methane concentration was closely related to the presence of the catalyst. The flow and diffusion had an important effect on the methane concentration. This model also predicted the outlet concentrations for ozone decomposition, which increased with increasing gas velocity. Interphase mass transfer was presented as the limiting step for this system. This structure-based mass-transfer model is important for the industrial application of TFBs.

Introduction

Fluidized-bed reactors represent the heart of many industrial engineering processes. Because of their low amplitude of pressure fluctuation, vigorous gas–solid contact, good mass- and heat-transfer efficiency, and high conversion rate (Basu & Subbarao, 1986; Bi, Ellis, Abba, & Grace, 2000; Chaouki, Klvana, & Guy, 1999; Lee & Kim, 1989), turbulent fluidized beds (TFBs) have been widely used in many industrial processes, such as fluid catalytic cracking, particle drying, the methanol-to-gasoline process, and Fischer–Tropsch synthesis (Bi et al., 2000; Edwards & Avidan, 1986; Ege, Grislingås, & de Lasa, 1996; Ellis, Bi, Lim, & Grace, 2004; Gao et al., 2009). In the turbulent regime, both bubbles and clusters are intermittently continuous and discontinuous, which results in sufficient gas–solid mass transfer; however, less attention has been paid to gas–solid mass transfer in TFBs, particularly in modeling. A better knowledge is of significance to understand, estimate, scale up, and optimize TFB reactors (Syamlal & O'Brien, 2003).

There have been few reports on gas–solid mass transfer of fluidization, most of which have focused on the fast and bubbling regimes, but there are almost no publications available for TFBs. Many studies (Basu & Subbarao, 1986; Du, Fan, Wei, & Warsito, 2002; Kai, Imamura, & Takahashi, 1995; Wang, Yang, & Li, 2005) have indicated that the fluidized regime significantly affects gas–solid mass transfer. Venderbosch (1998) investigated mass transfer and gas–solid contact in TFBs by the mass transfer-controlled oxidation of CO and used a numerical technique with a cluster model to interpret the conversion data. Unfortunately, only the outlet conversion was studied in his work. Computational fluid dynamics has recently become a popular method to study mass transfer in fluidized beds because of its powerful calculation and dynamic simulation capability. Chalermsinsuwan, Piumsomboon, and Gidaspow (2009) used the concept of additive resistances and one-dimensional steady-state balance with kinetic theory to compute the mass-transfer coefficients. Kashyap and Gidaspow (2010) used kinetic theory to compute the mass-transfer coefficient and

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Nomenclature

Symbols

a_c	Specific surface area of the cluster (m^2/m^3)
a_p	Specific surface area of the particle (m^2/m^3)
C_c	Gas concentration in the cluster phase (kg/m^3)
C_d	Gas concentration in the void phase (kg/m^3)
C_{Dc}	Drag coefficient in the cluster phase (dimensionless)
C_{Dd}	Drag coefficient in the void phase (dimensionless)
C_f	Average concentration of the gas active component in the calculating grid (kg/m^3)
C_{sc}	Gas concentration on the surface of particles in the cluster phase (kg/m^3)
C_{sd}	Gas concentration on the surface of particles in the void phase (kg/m^3)
C_0	Initial concentration of the gas active component (kg/m^3)
d_c	Equivalent diameter of the cluster (m)
d_d	Equivalent diameter of the void (m)
D_g	Mass diffusion coefficient of the gas (m^2/s)
f_c	Volume fraction of clusters
F_D	Drag force (N)
K_c	Mass-transfer coefficient between gas and solid in the cluster phase (m/s)
K_{cd}	Gas mass-exchange coefficient between the void phase and the cluster phase (m/s)
K_d	Mass-transfer coefficient between gas and solid in the void phase (m/s)
K_v	Constant of reaction rate (s^{-1})
M_{cd}	Mass transferred from the gas in the cluster phase to the gas in the void phase $(kg/(m^3 s))$
M_{inc}	Mass of the active component that enters the cluster phase in the element slice $(kg/(m^3 s))$
M_{ind}	Mass of the active component that enters the void phase in the element slice $(kg/(m^3 s))$
M_{outc}	Mass of the active component that exits from the cluster phase in the element slice $(kg/(m^3 s))$
M_{outd}	Mass of the active component that exits from the void phase in the element slice $(kg/(m^3 s))$
M_{pfc}	Mass transferred from the surface of particles in the cluster phase to the gas in the cluster phase $(kg/(m^3 s))$
M_{pfd}	Mass transferred from the surface of particles in the void phase to the gas in the void phase $(kg/(m^3 s))$
U_{fc}	Superficial gas velocity through the clusters (m/s)
U_{fd}	Superficial gas velocity through the voids (m/s)
U_{pc}	Superficial particle velocity in the clusters (m/s)
U_{pd}	Superficial particle velocity in the voids (m/s)
V_{pc}	Particulate effective volume of the cluster phase in the unit volume of the system (m^3/m^3)
V_{pd}	Particulate effective volume of the void phase in the unit volume of the system (m^3/m^3)
$x_{a,c}$	Mass fraction in the gas of the cluster phase
$x_{a,d}$	Mass fraction in the gas of the void phase
$x_{a,sc}$	Mass fraction on the surface of the particle in the cluster phase
$x_{a,sd}$	Mass fraction on the surface of the particle in the void phase

Greek symbols

β	Drag coefficient $(kg/(m^3 s))$
ε_c	Voidage of clusters
ε_d	Voidage of voids
ε_f	Voidage of the calculating grid
η	Internal diffusion effectiveness factor of the catalyst
ρ_f	Density of the gas (kg/m^3)
ρ_p	Density of the particle (kg/m^3)
ρ_b	Bulk density (kg/m^3)
μ_f	Viscosity of the gas (Pa s)

Subscripts

c	Cluster phase
d	Void phase
f	Fluid
p	Particle

Sherwood numbers in fluidized beds, but the axial component distribution, which is necessary to evaluate the reactor performance, was not obtained in this work. Dong, Wang, and Li (2008a) established a multi-scale mass-transfer model for gas–solid riser flows based on the extended work of the energy-minimization multi-scale model. Vepsäläinen, Shah, Ritvanen, and Hyppänen (2014) proposed a one-dimensional steady-state fluidized-bed model with bubble and emulsion phases to derive the interphase mass transfer in the bubbling and turbulent regimes. Liu, Wang, Zhang, and Li (2015) proposed a structure-dependent model by considering the dense–dilute structure, and applied heterogeneity indexes to simulate the mass transfer and reactions in fluidized beds.

It has been proven that voids and clusters of various shapes and sizes are the main characteristics in TFBs (Venderbosch, 1998; Yerushalmi & Cankurt, 1979) and play a significant role in successful simulations (Chalermsinsuwan et al., 2009; Chen, Li, Lv, & Zhu, 2015; Gao et al., 2008, 2009). Furthermore, replacing the particle diameter with the cluster diameter can effectively improve the mass-transfer prediction in fluidized beds. Nevertheless, the effect of the interphase mass transfer in each calculating grid and variation of cluster sizes are commonly ignored in many models (Dong et al., 2008a; Gao et al., 2008; Venderbosch, 1998; Wang et al., 2009), which limits their application. Mass-transfer models based on the local structure for fast (Hou et al., 2013) and bubbling fluidized beds (BFBs) (Lv, Li, Zhu, Li, & Zou, 2016) have been proposed; however, experimental evidence (Horio, Ishii, & Nishimuro, 1992; Lim, Zhu, & Grace, 1995; Yerushalmi & Cankurt, 1979) indicated that the phase continuity in the turbulent regime differs from that in the bubbling or fast regime, which means that these mass-transfer models cannot be directly applied to TFBs. A structure-based mass-transfer model is hence required for TFBs.

Considering the existence of voids and clusters, a mass-transfer model for TFBs was established according to mass conversation and the balance between reaction and mass transfer for each phase in this work. For the numerical simulation, the mass transfer required more variables than the hydrodynamics, so five parameters (C_c, C_{sc}, C_d, C_{sd}, C_f) were used to describe the mass transfer in this model. The flow parameters were solved using the structure-based drag model (Chen et al., 2015). This model was coupled with reactions and verified against experimental data, and the mass transfer in TFBs then analyzed.

Structure-based mass-transfer model

The local structure of TFBs consists of the cluster phase, void phase, and interphase. Particles are thought to be homogeneously distributed in both the cluster and void phases. The interphase, which is the single layer of particles on the surface of the cluster phase, i.e., the two-phase boundary layer, can be divided into two equal parts: the cluster phase and the void phase. Five param-