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Short Communication

Modeling study of gas-liquid mass transfer enhancement by cylindrical catalyst particles

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ABSTRACT

In this work, the influences of non-spherical catalyst particles on the enhancement of the gas-liquid mass transfer are numerically studied. The 3D unsteady diffusion-reaction equation both in the liquid phase and the solid catalyst particles is solved. A pseudo-homogenous model is employed as well. It is found that the SV cylindrical particles increase enhancement factor while SRSV cylindrical particles decrease it in comparison with the corresponding spherical particles. The horizontal cylinder and the vertical cylinder show small differences. The enhancement factor increases with catalyst concentration, rate coefficient of reaction and decreasing particle size. The data of pseudo-homogenous model agree well with the corresponding results of the fully resolved simulations.

1. Introduction

Gas-liquid mass transfer plays a crucial role in determining the performance of slurry reactors for numerous industrial applications. It is widely known that the rate of gas-liquid mass transfer can be enhanced by the presence of small solid catalyst particles in the liquid, which catalyze chemical reactions between the dissolving gas and a component of the liquid (Holstvoogd et al., 1988; Nagy, 1995; Nagy and Moser, 1995; Ruthiya et al., 2005).

The previous modeling studies are overwhelmingly based on the continuum approach, where the one or two dimensional steady state diffusion-reaction equation was solved (Ramachandran, 2007). The diffusion-reaction process inside the catalyst particles was usually not considered, though in some cases the influence of internal diffusion was taken into account by using the effectiveness factor. However, the complex gas-liquid-solid interactions and the chemical reactions taking place inside the solid particles would cause the spatial concentration gradients in every direction, not only perpendicular to the gas-liquid interface.

With the rapid development of computer hardware and numerical method, the effect of the solid particles on the gas-liquid mass transfer near the gas-liquid interface can now be investigated in more detail by fully resolved numerical simulation. Wenmakers et al. (2016) studied the enhancement of gas-liquid mass transfer due to a first order heterogeneously catalyzed reaction by means of 3D unsteady numerical simulations. Only spherical catalyst particles were modeled in their work nevertheless.

On the other hand, the pseudo-homogenous model is widely used in industry and be of high relevance to chemical engineers for a fast and first-level analysis. Wenmakers et al. (2016) also showed that the pseudo-homogeneous model produced comparable results with those of detailed numerical simulations. However, how the gas-liquid mass transfer is affected by non-spherical particles and whether the pseudo-homogeneous model can be applied to slurry systems with non-spherical catalyst particles are significant but still unresolved problems. As non-spherical particles are far more frequently encountered in industry, it is thus highly desired that further study is carried out to clarify the effect of non-spherical particles. Therefore, this work aims to fill in this gap, which is expected to make a relevant additional contribution.

2. Numerical model

2.1. Fully resolved model

This work targets to model the diffusion of the gas into a liquid film filled with small catalyst particles (the dashed box in Fig. 1), which can be seen as a small part of a gas-liquid interface neglecting the curvature.

The diffusion-reaction of the gas from the gas-liquid interface into the solid-liquid suspension is described by

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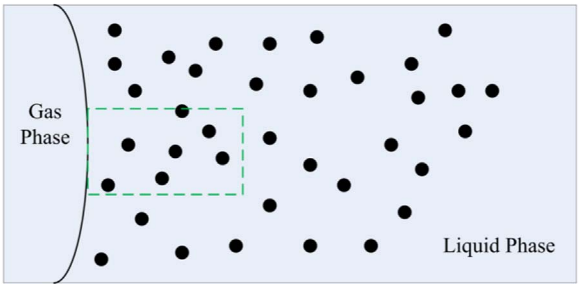


Fig. 1. Schematic representation of the gas-liquid interface.

$$\frac{\partial C}{\partial t} = \nabla\cdot(D\nabla C) - k_r C \tag{1}$$

where C is concentration, D is D_l for the liquid continuous phase and D_p for the solid particles. The first-order chemical reaction is modeled and only occurs in the solid particles while k_r=0 in the liquid phase.

2.2. Pseudo-homogeneous model

The pseudo-homogeneous model does not distinguish liquid phase and solid particles, and a homogeneous medium is assumed in where chemical reaction occurs. The material properties of the assumed homogeneous medium are constant throughout space. Its diffusion-reaction equation reads

$$\frac{\partial C}{\partial t} = D_{\text{eff}}\frac{\partial^2 C}{\partial z^2} - kC \tag{2}$$

where$D_{\text{eff}}$is the effective diffusion coefficient of the transferred gas species in the liquid-solid suspension (Wenmakers et al., 2016), k is the effective rate coefficient of reaction defined as

$$k = \eta k_r \varepsilon_p \tag{3}$$

where η is the effectiveness factor,ε_p is the total volume fraction of the particles.

For the first order kinetics, the effectiveness factor of spherical particle is (Levenspiel, 1999)

$$\eta = \frac{1}{\phi_s}\left(\frac{1}{\tanh(3\phi_s)} - \frac{1}{3\phi_s}\right) \tag{4}$$

where ϕ_s is Thiele modulus for sphere, defined as:

$$\phi_s = \frac{R_{\text{sph}}}{3}\sqrt{\frac{k_r}{D_p}} \tag{5}$$

The effectiveness factor of cylindrical particle is

$$\eta = \frac{1}{\phi_c}\frac{I_1(2\phi_c)}{I_0(2\phi_c)} \tag{6}$$

where I is Bessel function, and ϕ_c is Thiele modulus for cylinder, defined as:

$$\phi_c = \frac{R_{\text{cyl}}}{3}\sqrt{\frac{k_r}{D_p}} \tag{7}$$

The gas-liquid mass transfer enhancement is characterized by an enhancement factor (E), which is defined as the ratio of gas flux (J) into the liquid in case of a reaction and the gas flux into the liquid without a reaction (Westerterp et al., 1987):

$$E = \frac{\langle J_{\text{reaction}}\rangle|_{z=0}}{\langle J_{\text{noreaction}}\rangle|_{z=0}} \tag{8}$$

For the details of the pseudo-homogeneous model, please refer to Wenmakers et al. (2016).

3. Methodology

The computational domain is a rectangular box, which contains the continuous liquid and the solid catalyst particles. Two types of particle are used, one is sphere (the radius R_{sph}, the diameter $D_{\text{sph},}$ the volume $V_{\text{sph},}$ the external surface S_{sph}) and the other is cylinder (the radius R_{cyl}, the diameter is D_{cyl} and the height is equal to $D_{\text{cyl},}$ the volume V_{cyl}). For the cylindrical particles, two orientations are considered in reference to the z axis, i.e., vertical direction (hereinafter called vertical cylinder) and horizontal direction (hereinafter called horizontal cylinder).

In this work, the spherical particle is used as baseline and the sizes of the cylindrical particles are defined in two ways:

1). The cylindrical particle has the same volume as the spherical particle; thereby a volume diameter is used (hereinafter called SV cylinder):

$$D_{\text{cyl}} = 0.8736 D_{\text{sph}} \tag{9}$$

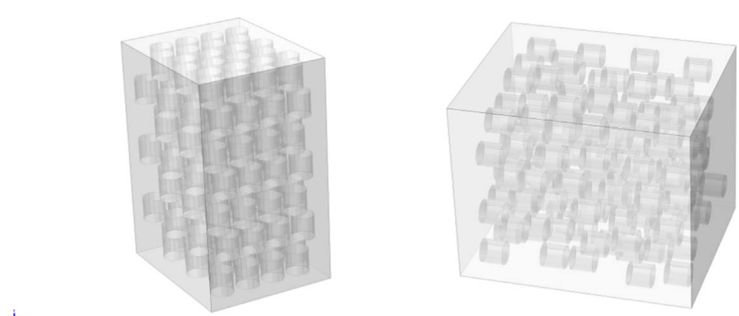
2). The cylindrical particle has the same ratio of external surface to volume as the spherical particle; thereby a Sauter's diameter is used (hereinafter called SRSV cylinder):

$$D_{\text{cyl}} = D_{\text{sph}} \tag{10}$$

Therefore, once the diameter of the sphere (50 μm, 100 μm) is defined, the sizes of the corresponding cylinders are automatically defined as described above and thus only the values of D_{sph} are specified in all cases.

Both random and hexagonal configurations of the particles are considered (Fig. 2).

The geometry is constructed using the MATLAB in-house code, and is transferred to the COMSOL 4.4 via MATLAB LiveLink. In the case of randomly configured particles, the dimensions of the rectangular box are $0.3\times0.3\times0.5\ \text{mm}^3$ for small particles and $0.8\times0.8\times0.5\ \text{mm}^3$ for large particles to ensure for a sufficient number of particles within the domain. In the case of hexagonally configured particles, the dimensions of the computational domain are determined by the number and size of particles, and the particle number ranges from 150–320.



(a) Hexagonal packing of vertical cylinders (b) Random distribution of horizontal cylinders

Fig. 2. Schematic representation of different particle configurations.