High-fidelity CFD modeling of particle-to-fluid heat transfer in packed bed reactors

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Abstract

The novel high-fidelity CFD model for packed bed reactors is validated in terms of *Nu* regarding particle-to-fluid heat transfer. The model is developed to take into consideration the flow of heat, mass and momentum through and around the particles each shaped without geometrical simplification. In the present approach, cylindrical shaped solid geometries are used to bridge particles in or near contact assuming the regions are stagnant. The bridges eliminate narrow gaps between particles and then enable treating hundreds of particles in the model. 220 of spherical particles are randomly packed in a cylindrical tube whose diameter is 4 times larger than particles. The predicted *Nu* is compared with a correlation, experiments and model predictions in the literature. In the smaller *Re* range, mesh independent solutions well agree with the literature. In the higher range, the applicable range varies from 200 to 700 depending on mesh density. Meshing strategy for increasing particle is rationally given by means of boundary layer theory.

Keywords: high-fidelity CFD model, packed bed reactors, heat transfer, DEM

1. Introduction

A packed bed is commonly used for catalytic reactions in petrochemical industry. For better understanding of the reactor, a computational fluid dynamics (CFD) has been applied assuming the bed can be regarded as a uniform porous media (Jakobsen et al., 2002). The assumption might be valid provided that the particle is significantly small compared to the reactor tube. If the reaction is extremely exothermic or endothermic, however, the narrow tube is utilized for achieving efficient heat transfer, in which the particle size is comparable to the tube diameter and hence the wall effect on the temperature and velocity would reach the center of the bed (Nijemeisland and Dixon, 2004). To resolve the situation, a high-fidelity CFD model has been recently developed, which constitutes a packed bed in a computational domain by generating spheres without geometrical simplification (Guardo et al., 2004; 2006; Nijemeisland and Dixon, 2004 and so on).

Although the geometrical simplification should be avoided as much as possible in the hi-fi CFD models, there is a need to treat contact points between particles in the bed. Since the contact point mathematically has no area, a numerical representation of it requires infinitely fine cells around it. Otherwise, highly skewed cells would be generated to fill the narrow gaps, which is undesirable numerically. In the most hi-fi CFD models, therefore, the contact points are eliminated by making the particles smaller or larger after initial arrangement of the particles in the bed. Even after the treatments, the fine computational cells are still needed in the space between shrunk particles or around the peripheral edge of overlapping face between enlarged particles. As the number of particles increases in the model, the necessity of fine cells immediately results in a large mesh size that cannot be handled easily. Further, the treatment can be implemented when particles are strictly in contact. If the distance between particles varies in the bed as can be seen in the randomly packed bed, the treatments might newly generate undesirably wide or narrow spaces. Consequently, the most hi-fi CFD models treated only tens of spheres packed regularly in a tube. For simulating a longer reactor tube, then, a periodic boundary condition is repeatedly applied to the shallow bed model in the axial direction (Nijemeisland and Dixon, 2004).

In the present study, the novel high-fidelity CFD model (Ookawara et al., 2007) is examined in terms of *Nu* regarding particle-to-fluid heat transfer in the bed. The model is developed for process intensification of packed bed reactors, which could be achieved for instance by blending catalytic and adsorbent particles in a bed (Xiu et al., 2003). In the model, cylindrical shaped solid geometries are used to bridge particles in or near contact assuming the contact regions are stagnant. Consequently, hundreds of particles in the random packing can be easily treated in the model. Although the effect of bridge on the flow properties can be negligible if the bridge is sufficiently within the stagnant region, the model should be carefully validated for its practical and reliable utilization. It is reported elsewhere (Ookawara et al., 2007) that the voidage of random packing, which is constituted by discrete element method, and the pressure loss through the bed, both well agree with the literature.

The predicted *Nu* is compared with a correlation, experiments and model predictions in the literature (Ranz, 1952; Wakao et al., 1979). Based on the comparison, discussed is the relation between prediction accuracy and mesh density. The meshing strategy will be given by means of boundary layer theory to increase the number of particles using a coarse mesh with sufficient accuracy.

2. CFD modeling and analysis

To verify the CFD and analytical procedure, the particle-to-fluid heat transfer is first evaluated for a single sphere suspended in a cylinder whose diameter and length are 7 and 16 times lager than the particle diameter. The inlet velocity of air with 300 K is varied in the particle *Re* ($=\rho U d_p/\mu$) range of 0.1 to 1000. The temperature of tube and particle are specified as 300 K (T_b) and 400 K (T_s), respectively. The tube wall is specified as moving in the flow direction at the inlet velocity of air to simulate infinitely uniform flow field. The *Nu* (=hd_p/k) is evaluated based on Eq. (1) by evaluating heat flux *q* through the particle surface.

$$q = h(T_s - T_b) \tag{1}$$

As shown **Fig. 1**, each coarse, medium and fine mesh examined in this study covers a particle with about 300, 1000 and 1500 of triangular surface cells, respectively. The volume mesh around the particle is generated from each surface mesh and hence the cell sizes are comparable. The mesh is not defined inside the sphere. The predicted *Nu* is compared with a well-know correlation Eq. (2) (Ranz, 1952).

$$Nu = 2 + 0.6\, Pr^{1/3}\, Re^{1/2} \tag{2}$$

Fig. 2 shows top and side views of the packed bed examined in this study. The random packing is constituted by a commercial code EDEM (DEM Solutions Ltd.), which is based on discrete element method. 220 of spherical particles whose diameter is 3 mm are randomly packed in a cylindrical tube whose diameter and length are 12 mm and 150 mm, respectively. The bed height is 52.3 mm and the voidage is 0.474. The size of original geometry constituted elsewhere (Ookawara et al, 2007) is reduced to one tenth in the computational domain for this study.

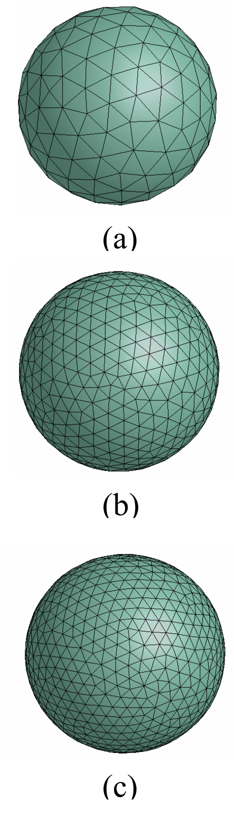

Fig. 1 Spheres covered by (a) coarse, (b) medium and (c) fine surface meshes.

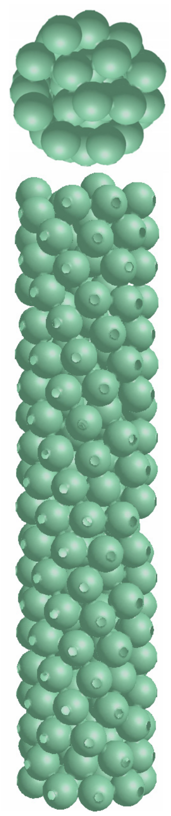

Fig. 2 Top and side views of packed bed

The inlet velocity of air with 300 K is also varied in the particle *Re* range of 0.1 to 1000. The temperature of tube and particles are specified as 300 K and 400 K (T_s), respectively. The *Nu* is again evaluated based on Eq. (1). In this case, the heat flux *q* is a mean value over the whole particles and the bulk-averaged temperature in the bed is taken as T_b. The film temperature (= $(T_s+T_b)/2$) is used to calculate the properties for evaluating *Re* and *Nu*. The *k*-*ε* model is employed as a turbulent model in the *Re* range above 300. The volume mesh in the packed bed is also generated from the particle surface with the three mesh densities aforementioned. The particle interior is out of the computational domain. The predicted *Nu* is compared with a correlation Eq. (3), experiments and model predictions in the literature (Wakao et al., 1979).

$$Nu = 2 + 1.1 Pr^{1/3} Re^{0.6} \tag{3}$$

All the CFD processes are performed by a commercial code FLUENT 6 (Fluent Inc.). The model of incompressible ideal gas for density, power law for viscosity and kinetic theory for specific heat and thermal conductivity are adopted, respectively.

3. Results and discussion

As an example, **Fig. 3** shows the temperature and velocity distributions around the single sphere in the cylindrical tube at *Re* = 10 obtained with the fine mesh. It can be seen that the thermal boundary layer around the sphere develops downstream. The extent of the domain, which is defined by referring to Guardo et al. (2006), seems to be sufficient to attaint the uniform flow field around the particle.

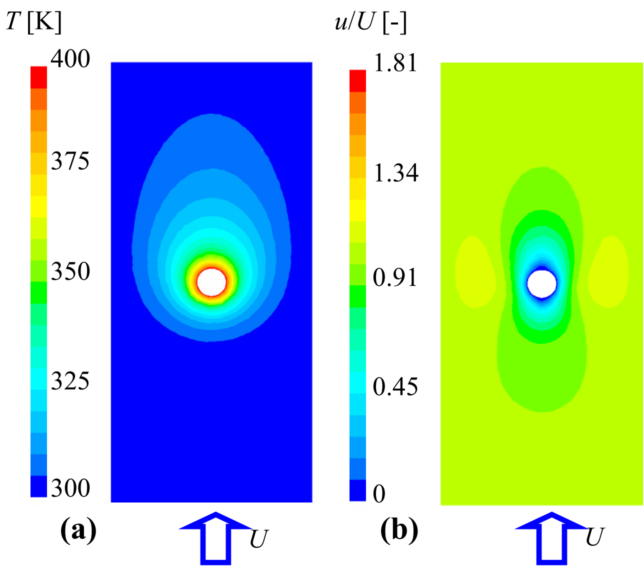

Fig. 3 (a) Temperature and (b) velocity distributions (*Re* = 10, fine mesh)

As shown in **Fig. 4**, the CFD-predicted *Nu* reasonably agrees with the correlation regardless of mesh density. Therefore, it can be concluded that these mesh densities are all sufficient for simulating heat transfer from a single sphere in the assumed infinite media in the examined *Re* range. In the case of single sphere, any turbulent model is not applied here since it is confirmed that the turbulent model does not significantly affect the results. The validity of the model is further to be considered in future.

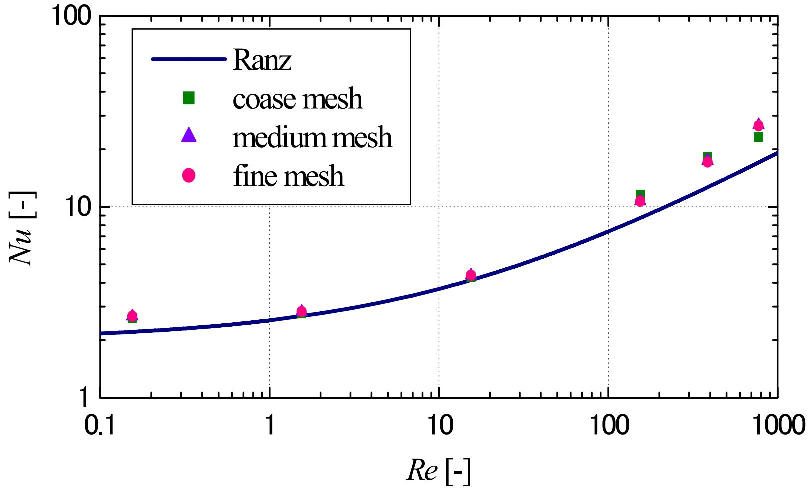

Fig. 4 Comparison of CFD-predicted *Nu* with a correlation

As an example, **Fig. 5** shows the temperature and velocity distributions in the bed at *Re* of 200 obtained with the fine mesh. It can be seen that the air temperature rapidly rises at first and afterwards remains high except near wall. The higher velocity occurs in the void extending in the flow direction, which is likely to exist in the random packing.

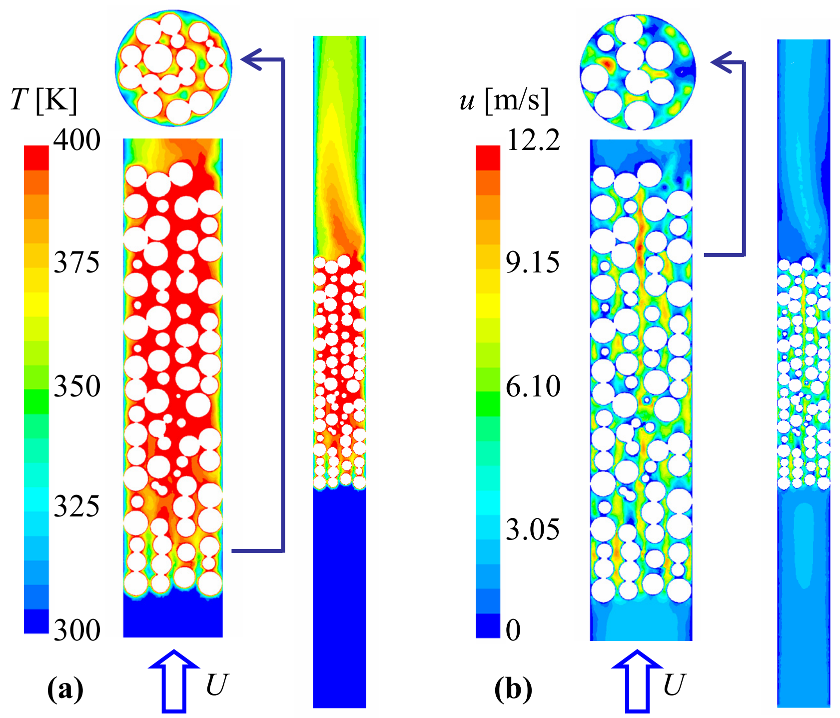

Fig. 5 (a) Temperature and (b) velocity distributions (*Re* = 200, fine mesh)

In the *Re* range less than 10, as shown in **Fig. 6**, the *Nu* converges to about 10 regardless of mesh density. It should be mentioned that previous model predictions at small *Re* also fell into the range of 10 to 18 in the literature (Gunn and De Souza, 1974; Pfeffer and Happel, 1964; Miyauchi, 1971). The *Nu* starts deviating higher from the correlation at *Re* of 100 and it approaches to 10 with a decreasing *Re*. The predicted trend is apparently similar with the experimental results. In the higher *Re* range, the applicable *Re* within 15 % deviation from the correlation varies from 200 to 700 depending on the mesh density. The higher mesh density apparently gives a better fit to the correlation.

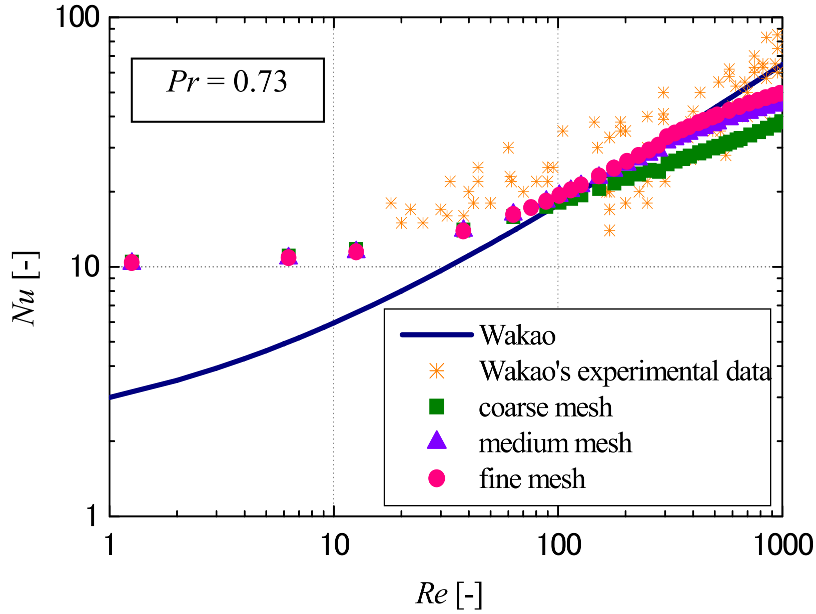

Fig. 6 Comparison of CFD-predicted *Nu* with the correlation and experimental results

The appropriate mesh density for a given problem is often determined by searching a mesh-independent solution. The procedure is rather tedious and even not rational. On the other hand, it is desired that the numerical model could contain the particles as much as possible in a bed at a reasonable computational cost so that the realistic CFD analysis would be performed easily. Therefore, it is of practical interest to predict a minimum mesh density with sufficient accuracy based on a theoretical background.

In the present study, the accuracy is related with a thickness of boundary layer, which is expediently assumed to form uniformly around the particle despite the complexity of flow field in the bed. It is further assumed that the accuracy is guaranteed provided that a volume cell exists within the thinner one of momentum and thermal boundary layers. When the height of computational cell on the particle surface is less than the thickness of boundary layer, the above condition is regarded to be satisfied. If there can be defined more than one cell within the thickness of boundary layer, of course, the accuracy is redundantly sufficient.

The definition of *Nu* for the sphere is expressed as;

$$Nu = \frac{hd_p}{k} \tag{4}$$

Similarly with the momentum and thermal boundary layers developing from an edge of thin plate, it is assumed that twice of heat transfer is occurred by convection compared with that caused by conduction. This is expressed by using a thickness of thermal boundary layer δ_T as;

$$\frac{h\delta_T}{k} \approx 2 \tag{5}$$

The Eqs. (4) and (5) immediately give a relation;

$$\delta_T = \frac{2d_P}{Nu} \tag{6}$$

Since *Pr* of air is about 0.73 in this study, it is assumed that the momentum boundary layer becomes thinner than the thermal boundary layer and the relation between these thicknesses follows;

$$\frac{\delta_M}{\delta_T} = Pr^{1/3} \tag{7}$$

Thus, a thickness of momentum boundary layer δ_M can be estimated from *Nu*.

On the other hand, the cell height is estimated from the average area of surface cell, which is calculated from the surface area of sphere and the number of cells covering it. The assumption that the volume cell is a regular tetrahedron immediately gives the cell height.

Table 1 lists the cell height on the particle surface for each mesh density and the thickness of momentum boundary layer δ_M, which most agrees with the cell height among the simulated conditions. The value of *Re* is the condition that gives the *Nu* related to δ_M.

Table 1 Cell height for each mesh density and a thickness of momentum boundary layer determined hypothetically at a given *Re* condition.

	cell height [mm]	δ_M [mm]	*Re*
coarse mesh	0.381	0.382	40
medium mesh	0.209	0.211	205
fine mesh	0.170	0.163	310

As can be seen in **Fig. 7**, the simulations with coarse and medium meshes deviate from mesh-independent solutions at the given *Re* above. Further, the predictions with fine mesh also deviate from the correlation given by Wakao (1979) at the *Re*. It should be noticed that the deviations are always downwards, which means the heat transfer is underpredicted. This is reasonably because the boundary layer cannot be appropriately described in the simulations due to the lack of mesh density in the region. It can be concluded, therefore, that the present hypothetical approach could rationally give an appropriate mesh density at any *Re*. The method is useful both to increase *Re* with a necessary fine mesh and to increase the number of particles with a minimum mesh density.

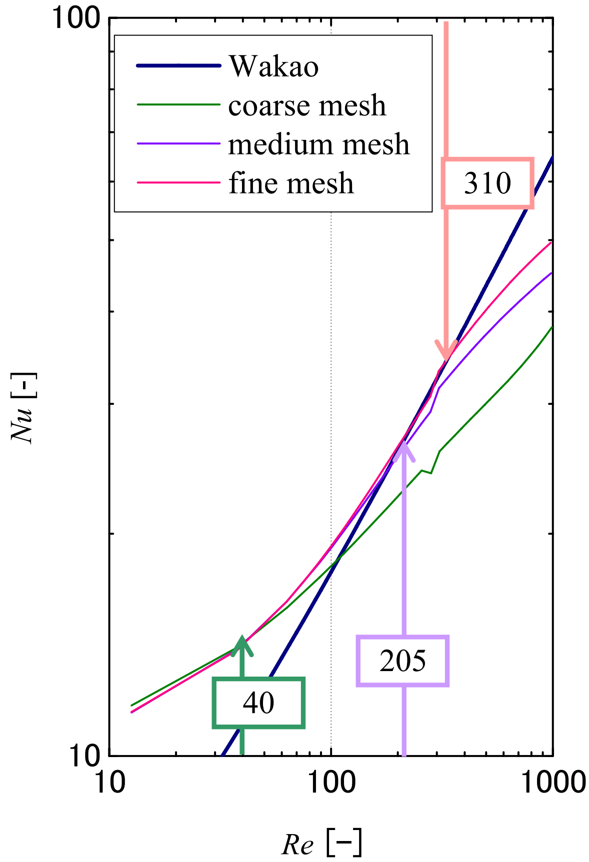

Fig. 7 *Re* conditions for each mesh density to predict the accurate heat transfer.

4. Conclusions

The novel high-fidelity CFD model associated with the interparticle bridge model (Ookawara et al., 2007) is validated in terms of particle-to-fluid heat transfer in a packed bed. The CFD-predicted *Nu* is compared with the correlation, experiments and model predictions for packed beds in the literature. In the lower *Re* range, the predicted trend is apparently similar with the experimental results and model predictions regardless of mesh density. In the higher *Re* range, the applicable *Re* within 15 % deviation from the correlation is 700 with the finest mesh.

It is shown that a minimum mesh density to assure the prediction accuracy could be given at any *Re* based on the assumed relation between thickness of momentum boundary layer around the spheres and cell height on the particle surface. It should be emphasized that the present hypothetical approach is useful to increase the number of particles by keeping the mesh density minimum with a sufficient accuracy, which leads to a large-scale of and thus practical modeling of packed bed reactors.

Acknowledgments

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