Effect of Particle Shape Features on Fluid Flow and Heat Transfer Characteristics using Particle-Resolved CFD Simulations

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Highlights

- Relationship between particle shape features and flow and heat transfer performance.
- Heat transfer performance is not solely dependent on particle surface area.
- Optimization of particle shape for enhanced bed performance i.e., lower ΔP and higher heat transfer.

1. Introduction

Packed bed reactors (PBRs) are extensively utilized in the chemical industry for solid-catalyzed gas-phase reactions (e.g., methanol steam reforming, CO_2 conversion, methanol synthesis, etc.). In recent years, there have been significant research efforts on particle-resolved CFD (PR-CFD) simulations for understanding solid-catalyzed gas-phase reactions at the particle-scale. This involves a comprehensive analysis of fluid flow, heat, and mass transfer limitations. Due to its profound impact on the local flow field, the shape of particles plays an important role in designing and optimizing PBR. The performance of PBRs can be enhanced by analyzing the relationship between particle shape and particle-scale fluid flow, and therefore, understanding the heat and mass transfer characteristics. Several researchers have investigated the effect of particle shape on flow and heat transfer characteristics. There is significant potential in optimizing particle shapes and innovating new shapes using the PR-CFD simulations. Therefore, it is important to establish the role of specific particle features in both the particle-scale flow and heat transfer characteristics. In the present study, several new particle shapes with internal intrusions, external intrusions and a combination of these two are investigated. In view of this, the objectives of the present work are (a) to investigate effect of particle shape on flow and heat transfer characteristics, (b) to establish a relationship between particle features and heat transfer, and (c) to optimize particle shape to enhance the heat transfer characteristics.

2. Methods

To study the effect of particle shape on flow and heat transfer characteristics, a single string of 10 particles of different shapes [see Figure 1 (a)] is placed manually in a cylindrical tube [D = 27.6 mm, see Figure 1(b)]. In the present study, internally- and externally-shaped particles (d_p and h = 20 mm) namely, external lobes with a hole, cylinder with parallel ribs, gear, Raschig ring with fins, pall ring, cylcut with fins, and cylinder with perpendicular ribs having the same particle volume are considered [see Figure 1 (a)]. The Reynolds-averaged continuity and Navier-Stokes equations are solved to simulate the fluid flow at Re_t of 50,000. Further, the Reynolds-averaged enthalpy equation is solved to simulate the conjugate heat transfer. The simulations are performed using Ansys FLUENT (v2021R1) on the high-performing computing facility of IIT Delhi, using approximately 120 cores in parallel. A single string of 10 particles is considered to investigate the effect of particle shape on flow and heat transfer characteristics. Further, for a few selected particle shapes with improved performance, multi-particle simulations of randomly generated packed beds with ~60 particles will be performed.

3. Results and discussion

To understand particle-scale fluid flow and heat transfer characteristics, PR-CFD simulations are performed in the bed of shaped particles. To mimic endothermic reaction conditions, a constant volumetric heat sink (equivalent to heat flux applied to the tube wall in Watts) is introduced in the solid domain. These simulations are carried out at high temperature (824 K) and high pressure (~21 bar) to comprehend industrially important solid-catalyzed gas-phase reactions. Figure 1 (c) shows velocity streamlines in the vicinity of particles. Notably, the bed of pall ring and cylinder with parallel ribs exhibits relatively higher velocities followed by cylcut with fins, Raschig ring with fins and subsequently, cylinder with parallel ribs, gear and external lobes with hole. In the case of pall ring, the presence of holes normal to the flow direction creates flow resistance in both radial and axial directions which leads to large backflow regions and consequently higher velocities within the bed. Similarly, in the cylinder with parallel ribs, these ribs are oriented normal to flow direction and continuously change the direction of flow, generating large backflow region around the particles leading to higher velocities in the bed. However, in all other particle shapes, the internal and external intrusions are aligned with the flow direction, hence they offer minimal resistance to flow resulting in lower velocities within their respective beds compared to pall ring and cylinder with parallel ribs. Pressure drop (ΔP) is analyzed across the bed after excluding one particle height from the top and bottom of the bed and shows higher ΔP in the bed of the pall ring followed by cylinder with parallel ribs [see Figure 2 (a)]. In these cases, holes and ribs are aligned normal to the flow direction attributed to the increased backflow regions and consequently higher ΔP. However, for all other particle shapes, ΔP remains comparable and significantly lower than pall ring and cylinder with parallel ribs, owning to the particle features aligning with the flow direction.

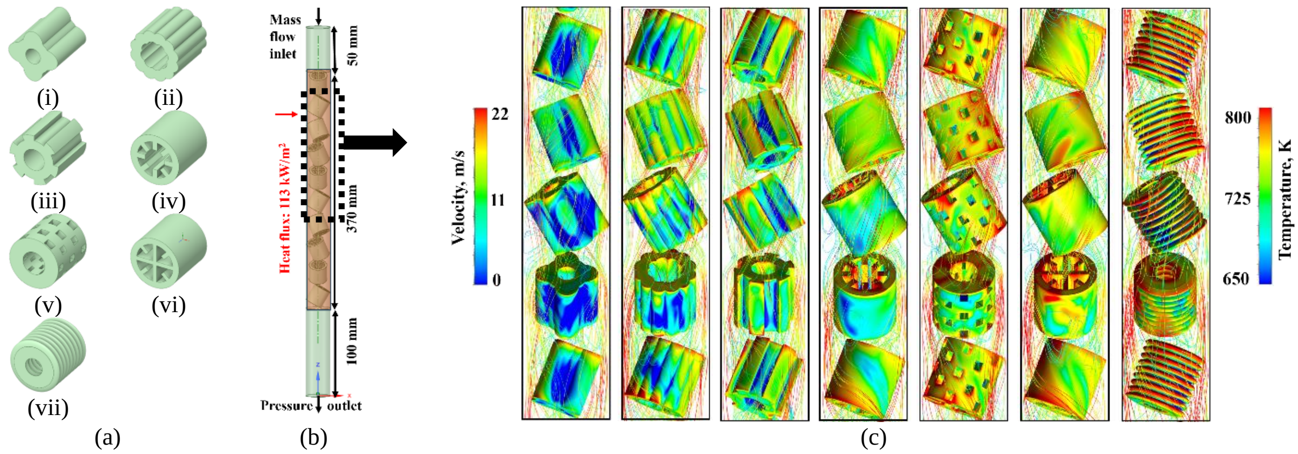

Figure 1. (a) Particle shapes, [(i) external lobes with hole, (ii) cylinder with parallel ribs, (iii) gear, (iv) Raschig ring with fins, (v) pall ring, (vi) cylcut with fins and, (vii) cylinder with perpendicular ribs], (b) computational domain with boundary conditions and (c) velocity streamline and surface temperature on the particle surface.

In addition, conjugate heat transfer simulations are also performed to understand temperature distribution within the bed of different particle shapes. Figure 1(c) shows the temperature distribution on the surface of particles for all cases. Qualitatively, Raschig ring with fins, pall ring, cylcut with fins, and cylinder with perpendicular ribs exhibit higher surface temperature compared to external lobes with hole, cylinder with parallel ribs, and gear. The enhanced heat transfer performance is attributed to the higher velocities around the particles leading to higher convective heat transport from fluid to particles. To evaluate the heat transfer behavior quantitatively, area-averaged surface temperature ($< T_s >$) and volume-averaged temperature ($< T_v >$) are investigated [see Figure 2 (b)]. The $< T_s >$ and $< T_v >$ are found in the order of cylcut with fins > pall ring > Raschig ring with fins > cylinder with perpendicular ribs > cylinder with parallel ribs > gear > external lobes with hole. Although cylinder with perpendicular ribs has a higher particle surface area as compared to cylcut with fins, it shows lower heat transfer performance indicating that heat transfer also depends on factors other than the particle surface area. The heat transfer performance of pall ring and Raschig ring with fins is relatively comparable, however a substantial difference in ΔP can be observed due to the specific particle features as discussed earlier (see Figure 2). These findings suggest the importance of specific particle features (such as wall thickness, hole size, orientation of ribs, etc.) which play a crucial role in enhancing heat transfer performance while maintaining a lower ΔP. Additionally, bed-scale simulations are performed for particle shapes depicting enhanced flow and heat transfer performance and compared with 7-hole cylinder particle shape. The computational domain of one such packed bed of cylcut with fins particles is shown in Figure 2 (c). Further details will be reported in the full-length manuscript.

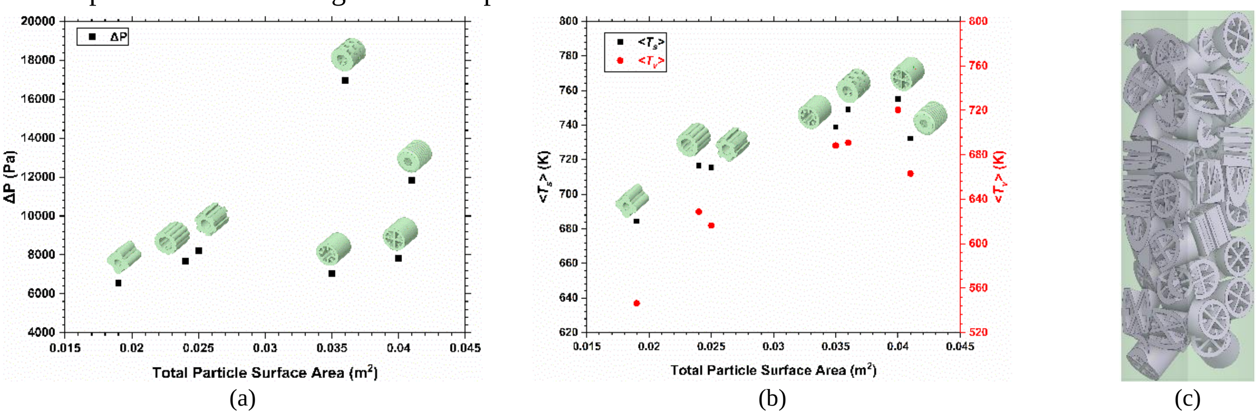

Figure 2. Effect of particle shape on (a) ΔP, (b) $< T_s >$ and $< T_v >$ and (c) computational domain of cylcut with fins particle shape.

4. Conclusions

In the present study, PR-CFD simulations are performed to investigate the effect of particle shape on flow and heat transfer characteristics. The pall ring exhibited higher velocities and ΔP, while cylcut with fins showed higher values of $< T_s >$ and $< T_v >$. From these findings, it is observed that heat transfer is not only governed by the surface area of a particle, rather it is found to be a function of the size of internal hole, wall thickness, internal and external intrusions. These findings highlight the importance of particle shape features (such as wall thickness, hole size, orientation of ribs, etc.) which are crucial for comprehending and optimizing heat transfer performance. Further, a detailed quantitative relationship between particle shape features and heat transfer performance will be provided in the full-length manuscript.

Keywords: Packed bed, shaped particle, particle-resolved CFD and heat transfer performance.