Evaluation of The Radial Void Fraction Distribution in Random Packing Structures of Non-Spherical Particles

Ali Farbod1*, E. M. Moghaddam2

1 Pooya Bod Raya Eng. Co., Mashhad, Iran; 2 Process & Energy Department, TU Delft, Leeghwaterstraat 39, Delft, The Netherlands

*Corresponding author: farbod@pouya3d.com

Highlights
- RBDPac code was employed to investigate the radial void fraction profile in non-spherical packings.
- The random packings of cylinders and rasching rings with different dimensional features were generated.
- The results demonstrate discernable differences between the local porosity profile of shaped particles.
- The influence of pellets’ aspect ratio and hole diameter on the oscillatory pattern of local voidage was investigated.

1. Introduction
Packed beds are extensively used in almost all chemical process industries. The most important use of such unit operations can be found in reaction engineering where they are employed as catalytic fixed bed reactors with either single or two-phase flow. In such units, catalytic particles can be exercised with different shapes, e.g. spheres, equilateral cylinders, pall rings, rasching rings, trilobes, and different sizes ranging from fine powders, often reaching several millimeters to catalyst pellets of around several inches. Virtually all models used in design of such systems take the role of bed structure into account in different specific ways. For example, classical plug flow models such as homogenous models use the bulk voidage, the simple versions of non-plug flow approaches, such as $\Lambda(r)$ model proposed by [1], employ radial void fraction distribution and more advanced approaches such as Computational Fluid Dynamics (CFD) technique exercises either radial proosity profile or the geometrical model representing the positions of particles in the bed. However, the majority of advanced design procedures has exerted the local bed porosity to track the influence of bed structure on spatial propagation of transport scalars in the reactor. This is because of the inadequacy of global properties, e.g. mean voidage and packing density, to reflect the influence of bed topology at the pellet scale, where the local changes in porosity can lead to large variations in velocity fields and accordingly radial heat loss and dispersion of mass along the bed [2]. This has persuaded researchers to deal with the prediction or measurement of the local bed porosity whereby, the radial porosity variations for mono-sized spheres in cylindrical containers are mainly addressed, e.g. [2,3,4]. Nonetheless, there are very few references that investigate the behavior of radial porosity in random packings of non-spherical particles, e.g. [5,6,7], where the patterns, i.e. the amplitude and the period of oscillations, are completely different comparing to spherical packings.

The main aim of this contribution is therefore to establish a basic understanding concerning the local properties of random packings of non-spherical particles, including solid cylinders with different aspect ratios, rasching rings with different hole diameters, using RBDPac Code [8]. Due to scarcity of published data on radial voidage profile of non-spherical particles, the prevailing data for spherical packings were used to validate the results of packing simulations. Furthermore, a conceptual strategy was proposed to obtain axially-averaged radial void fraction distribution from simulated structures, which not only is more accurate than the routine methods like arc-length approach, but also it is remarkably straightforward and time saving.

2. Methods
The random packings of different pellet’s shapes, including spheres, solid cylinders with different aspect ratios and rasching rings with different hole diameters were generated using RBDPac, which is a code developed based on the concept of Rigid Body Dynamics [8]. In the RBD simulations, both pellet-pellet and pellet-wall collisions were considered and modelled by impulse theory, and Coulomb friction model was also adopted to
implement frictional force upon collision, simultaneously. The objects’ collisions are detected through a hard-body approach, whereby the colliding contacts can be determined through point to mesh face as well as edge-edge contacts, where the objects are described by triangular polygons. Simulation data were given in Table 1.

In order to compute the axially-averaged radial void fraction profile, a planar polygon-based approach was adopted in which a simulated structure is intersected with a series of concentric tubes with different diameters (see Figure 1). The local voidage at specific radius can then be calculated by the following formula:

\[ e(r) = 1 - \frac{S_{\text{int}}}{S_{\text{total}}} \]

where \( S_{\text{int}} \) is the intersecting area with pellets and \( S_{\text{total}} \) is the area of tube that intersects the bed at radius \( r \).

3. Results and discussion

The results of packing simulations demonstrate the capability of RBDpac in generating random packings of non-spherical pellets (see Figure 2). Furthermore, postprocessing analyses show that there is a pronounced difference concerning the pattern, i.e. amplitude and wave length, between the radial porosity profile of spherical and cylindrical packings, and this difference is noticeably discernable for different. Furthermore, the influence of aspect ratio of solid cylinders, as well as hole diameters of rasching rings, on the oscillatory behavior of the local void fraction profile were systematically investigated.

4. Conclusions

The radial porosity distribution as well as the bulk porosity in a series of random packings of different shapes were computed using RBD method. The results demonstrate the capability of this approach in addressing structural properties of random packings of non-spherical packings.

References

Keywords
Packed Beds, Radial Void Fraction Distribution, Rasching Rings, Cylindrical Pellets, RBDPac

Table 1. Packing simulation data

<table>
<thead>
<tr>
<th>Objects’ Material: Stainless Steel (( p=8.03 \text{ gr/cm}^3 ))</th>
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<tbody>
<tr>
<td>Pellets’ Shape &amp; Size</td>
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<tr>
<td>Sphere (( d_p=10 \text{ mm} ))</td>
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<tr>
<td>Cylinder (1/( d_p=0.5,1,1.5 &amp; d_p= 10 \text{ mm} ))</td>
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<tr>
<td>Rasching rings (1/( d_p=1, d_h=0.2, 0.8,9.97 \text{ mm} &amp; d_p= 10 \text{ mm} ))</td>
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<tr>
<td>Bed size: ( d_t=35.5 \text{ to } 91.73 \text{ mm}, resulting in } 3.55\leq d_t/d_p\leq9.17 )</td>
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<tr>
<td>Friction Factor: 0.2 for pellets &amp; 0.6 for tube wall</td>
</tr>
<tr>
<td>Surface Bounciness: 0.9 for pellets &amp; 0.6 for tube wall</td>
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</tbody>
</table>

Figure 1. Radial void fraction profile of rasching ring packing with \( d_t/d_p=5 \), computed using polygon-based radial method

Figure 2. Random packings of particles of different shapes with \( d_t/d_p=7 \)