Numerical Parameter Study on Bed Porosity of Random Packed Beds of Spheres

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Highlights

- Generation of random packings using open-source software blender™ and LIGGGHTS®.
- Influence of material properties and packing characteristics on bed porosity are shown.
- Raise awareness towards software choice and parameter settings for packing generation.

1. Introduction

Fixed bed reactors are commonly used in the chemical industry for heterogeneous and multiphase reactions. The conversion strongly depends on the fluid flow across the reactor which, in turn, is affected by the local porosity inside the reactor, in particular, due to the pressure drop and the heat management. Various authors have attributed their work to characterising random packings of spherical particles in cylindrical confined walls, both experimental and numerical. The cylinder-to-particle diameter ratio is identified as having a significant influence on bed porosity. The influence of other factors is indicated such as particle density [1], packing mode and particle surface roughness [2], particle shape [3], inter-particle and wall friction [4] as well as restitution [5]. Nonetheless, a comprehensive analysis of the numerous factors influencing the porosity of packed beds could not be found in literature.

Since uncertainties in the bed porosity entail errors in the flow characteristics and conversion of catalytic fixed-bed reactors, an attempt is made to characterise the influence of material properties and packing characteristics on bed porosity using numerical simulation.

2. Methods

Packed beds of monosized spherical particles in cylindrical confined walls are generated using two open-source software packages, blender™, utilising rigid body dynamics by integrating the Bullet physics library, and LIGGGHTS®, applying the discrete element method. In addition to local porosity profiles, the mean packing porosity of the resulting beds is evaluated whereby sections with a height of four times the particle diameter at the bottom and of three times the particle diameter at the top of the backed bed are omitted to exclude the ordered bed at the bottom and incomplete layers of particles on top of the packing respectively.

Parameter studies to characterise the influence of material properties such as density, friction and restitution as well as packing characteristics namely number of particles, bed height related to particle diameter and cylinder-to-particle diameter ratio on the bed porosity are conducted for both approaches and compared.

3. Results and discussion

Although not shown here for brevity, the local porosity profiles of the simulated packings yield the expected patterns and the mean bed porosities are within the expected range for loose random packings. In Figures 1 and 2 the influence of friction and restitution on the mean bed porosity are depicted for two cylinder-to-particle diameter ratios (D/d) using both software packages. Here, either the coefficient of friction (COF), the coefficient of restitution (COR) or both are varied while other settings remain unchanged. Two general trends can be observed: bed porosity increases with increasing coefficient of friction and bed porosity decreases for high values of restitution. Superimposing both effects shows that porosity is dominated by friction for low values of the coefficients of friction and restitution whereas the effect of restitution is visible at high values. A comparison of two packings with different cylinder-to-particle diameter ratios, both simulated with LIGGGHTS®, is shown in Figure 3. The bed porosity as function of friction is shifted to higher values for the lower cylinder-to-particle diameter ratio. In the same figure differences in the results obtained with blender™ and LIGGGHTS®are revealed. This may be due to simplifications used in the rigid body approach, but further investigation is required. Still, both software packages show similar trends for the exemplarily chosen parameters.

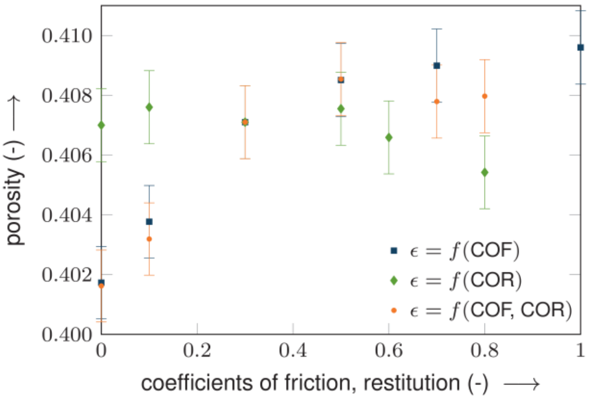

Figure 1. Influence of friction and restitution on bed porosity for packings with D/d = 7.35, simulated with blender™.

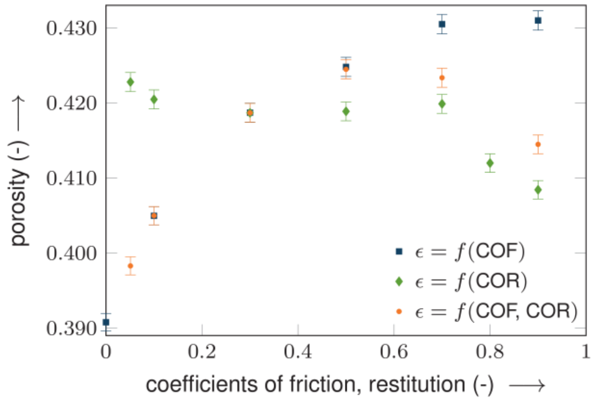

Figure 2. Influence friction and restitution on bed porosity for packings with D/d = 8.41, simulated with LIGGGHTS®.

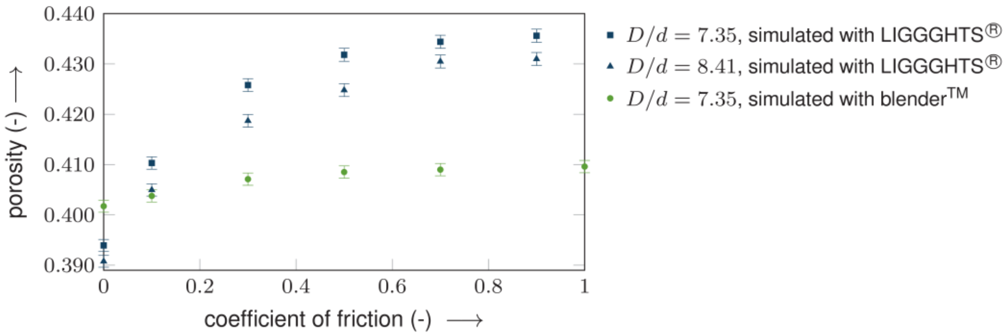

Figure 3. Influence of friction on bed porosity for different D/d ratios and comparison between software packages.

4. Conclusions

Both applied software packages are capable of simulating random backed beds of spherical particles to a certain extent. The resulting packed beds show variations in their mean porosity as a function of different parameters. The influence of some of the shown parameters is of such significance that they cannot be neglected in the numerical packing generation without introducing high potential errors propagating through possible subsequent CFD simulations. Hence, simply letting spheres drop into a cylinder without through consideration of the parameters involved might not be sufficient. It is strongly recommended to pay special attention to the parameter selection for packing generation by means of numerical simulation in addition to the choice of simulation software.

References

[1] R. Rutgers, Nature 193 (1962) 465–466.
[2] A. de Klerk, AIChE Journal, 49 (2003) 2022–2029.
[3] F. Benyahia, K.E. O'Neill, Part. Sci. Technol. 23 (2005) 169–177.
[4] J. Theuerkauf, P. Witt, D. Schwesig, Powder Technology 165 (2006) 92–99.
[5] J. Pottbäcker, O. Hinrichsen, Chem. Ing. Tech. 89 (2017) 454–458.

Keywords
numerical packing generation; bed porosity; material properties; open-source software.