Numerical modeling of random packed beds of various packing densities with a sequential deposition algorithm

Maciej Marek

Faculty of Mechanical Engineering and Computer Science, Częstochowa University of Technology, Częstochowa, Poland

Corresponding author: marekm@imc.pcz.czest.pl

Abstract. The algorithm presented in this work allows for numerical generation of the geometry of a random packed beds of cylinders, Raschig rings and Intalox saddles. During the simulation, based on a simplified mechanics of the filling process, the particles are dropped sequentially into a cylindrical container. Various packing densities are obtained depending on the magnitude C_F of the artificial radial force. It has been shown that the results are sensitive to C_F only when its value is much smaller than gravity and realistic porosity is obtained for C_F comparable or larger than gravity.

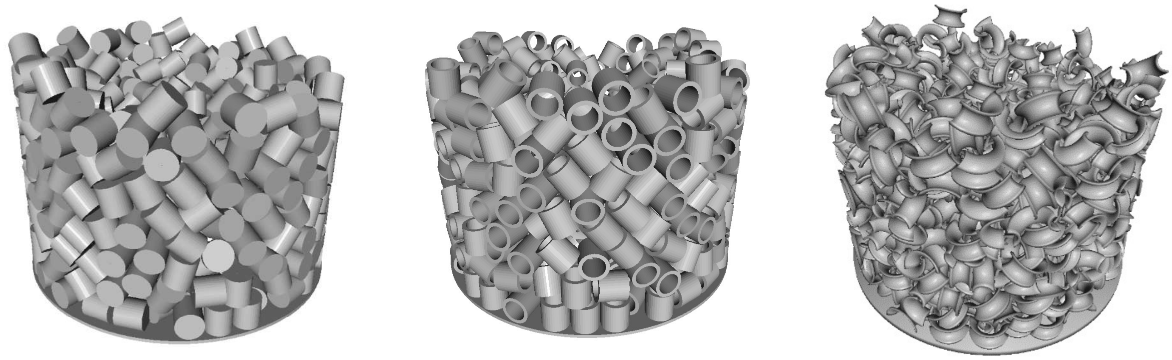
INTRODUCTION

Numerical generation of random packings of non-spherical particles is a non-trivial task. The model should provide the final structure of non-overlapping particles with realistic packing density but even when the distribution of porosity is correctly reproduced orientations of particles may not be valid [1]. In the literature there are many approaches to generation of packed beds including Monte Carlo or optimisation methods but the most promising seem to be ones in which Newtonian mechanics is applied to motion of individual particles – DEM (Discrete Element Method) [2]. However, the problem with DEM is computational complexity, especially for large beds when motion of many particles has to be solved during the course of the whole simulation. The algorithm proposed in [3] allows for sequential deposition of particles and keeping the rest of the bed "frozen" which greatly facilitates the computational process and simplifies the method. Although methods of this type have been known to provide rather low packing densities [4], the current algorithm is free from this disadvantage due to inclusion of an artificial radial force [3] and, moreover, reproduces orientation of cylindrical particles with a good accuracy [5]. The geometry of a numerically generated packed bed of Raschig rings has been previously used in CFD simulation of a flow in a chemical catalytic reactor [6].

NUMERICAL MODEL AND SAMPLE RESULTS

The motion of a particle is influenced by physical forces – gravity, reaction forces from other particles and container's walls – and artificial force directed normal to the container's axis (radial force). The particle is placed in a random position above the bed, drops until the mechanical equilibrium is reached (with radial force turned off), then the radial force is activated and after another equilibrium state the particle drops again with only physical forces active. When at rest, the particle is incorporated into the bed structure and remains there with its position and orientation fixed until the end of the simulation. The reaction force depends on the overlap between the particles. The overlap is easily calculated as the active particle is covered with a mesh of markers and the problem is reduced to finding immersion distance of a point in the other particle. The details of the method are presented in [3] (cylinders) and [6] (Raschig rings). Here this methodology is extended to Intalox saddles. Sample beds are shown in Fig. 1.

The main results of the present work include: a) dependence of the global and local bed porosity on the magnitude C_F of the radial force (Fig. 2, left); b) sensitivity analysis of the porosity distribution to C_F; c) dependence of the particle orientation distribution to C_F (Fig. 2, right). It has been shown that the algorithm allows for tuning the parameter C_F in order to obtain required packing density (global porosity in the interval 0.38-0.46). The maximum packing density is attained for C_F comparable to gravity G and increasing this parameter further has negligible influence on the bed structure, which is the most sensitive to C_F in the interval 0-0.01G. As for the orientation distribution, its character is significantly different for loosely and densely packed particles. In the former case, the distribution has a broad peak near 55°, while in the latter case – a distinct maximum at 90°.



(a) (b) c)

FIGURE 1. Sample beds generated with the algorithm: a) cylinders, b) rings, c) saddles

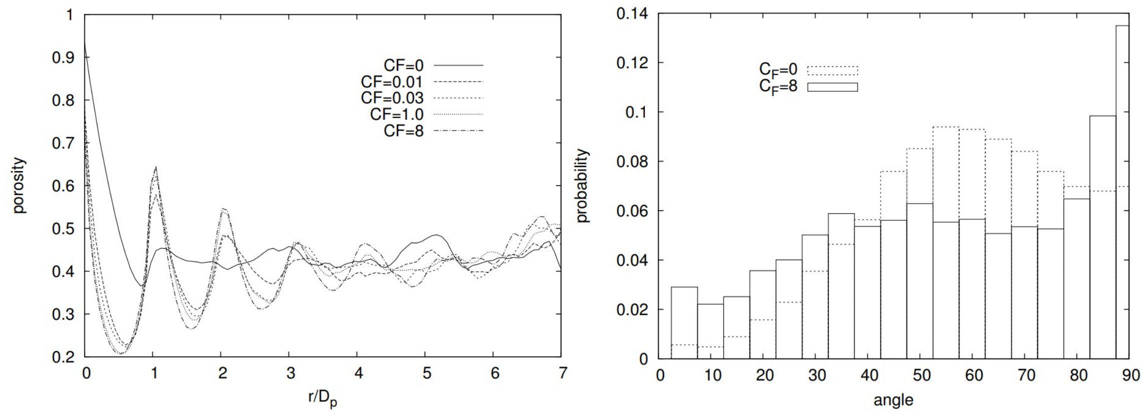


FIGURE 2. Radial porosity profile (left) and particle orientation distribution for different magnitudes C_F of the radial force (right). Notation: r – distance from the container wall, D_p – diameter of the particle

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