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Simulation and characterisation of packed columns for cylindrical catalyst supports and other complex-shaped bodies

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Abstract. Catalyst pellets are packed in reactor beds and the shape and mechanical properties have a major influence on the reactor performance by virtue of (i) the detailed topology of the void space and grain surface area and (ii) the fragility of the pack to withstand in-service stresses within the solid skeleton – often through thermal and cyclic stressing. The paper highlights the features of the FEMDEM code used to simulate these performance-related properties of the pack. The local porosity, packing structure, bulk porosity and orientation distributions of the resulting bodies making up the pack of pellets will be presented. The generic methodology illustrated is shown to be suitable for shape optimisation of industrial packing processes.

Keywords: FEMDEM, complex-shaped bodies, packed columns, simulations.

1 Introduction

FEMDEM numerical simulations of multi-body systems can be applied to any type of body geometry and their results can be employed for the characterisation of the system of particles, such as local porosity, packing structure, bulk porosity, and orientation distributions of the resulting bodies making up the pack of pellets.

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An example is the characterisation of the packing performances of catalyst supports, i.e. the ceramic pellets where the actual catalytic metal is dispersed, which are employed in fixed bed reactors. During the standard lifecycle of the plant some of the ceramic pellets are crushed to fragments due to the thermal contractions of the reactors, reducing their service life and their efficiency. In particular, the accumulation of fine fragments may produce localised reductions of permeability in the reactor, causing pressure drops and potentially reducing the lifetime of the reactor itself. Ultimately more realistic loading conditions, such as the force chains and the consequent compression applied by neighbouring catalysts due to the thermal shrinkage of the reactor, can be evaluated for an even more precise understanding of mechanical solicitations applied to a catalyst supports before failure.

In (1) it has been shown how FEMDEM simulations can be employed for the evaluation of the mechanical performance of catalysts to improve their strength and reduce the number of fine fragments at failure while meeting the required geometric surface area. The problem of simulating the packing of cylindrical bodies in a cylinder has been approached with numerous computational techniques in the literature. In (2) the packing process is simulated with both a semi-stochastic approach, where the particle path is randomly determined on the base of the overlapping of voxels, and a deterministic approach, where the repulsive forces and torques applied to the particles are calculated by measuring the number of their overlapping voxels and their voxel-level contact forces. In (3) these voxel-based methods are compared to discrete-element simulations where the contact forces are calculated between pairs of spheres and the pellets are represented with clusters of spheres clumped together. In this work some of the advantages of FEMDEM in modelling multi-body interactions for ceramic materials is presented. These include the potential to represent not only cylindrical pellets, but any complex-shaped body, such as tridecagram-shaped particles. Experimental and numerical results are compared, in particular FEMDEM numerical simulations of packing of cylindrical catalyst supports in a cylindrical container are compared to the corresponding experimental results from X-Ray CT scans.

2 Numerical Simulations

FEMDEM simulations have been employed to simulate pellets being cast into a cylindrical container: the bodies are discretised with a tetrahedral mesh and their contact forces are calculated with a penalty method and a Coulomb model of friction. The energy loss during the impacts is modelled with a damping force proportional to the particle velocity during the impact. The geometries of the container and the cylindrical catalyst support (A38) refer to (2) and have been imported from CAD drawings. The particles are introduced in the domain above the container base in layers of forty-nine pellets each, from a fixed height, with random

orientations and zero initial velocity. This process is completely automated through POSITIT, a pre-processing tool that facilitates the control of filling conditions and avoids the need for a manually defined 3D space for the initial conditions of each single pellet. The simulation runs in parallel on ten cores in less than twenty-four hours. The numerical results are then analysed with a post-processing tool (PORO) to estimate the axial and radial packing density profiles and the pellet orientation distribution.

2.1 Model Definition

A 44.5 mm inner diameter cylindrical container is filled with more than three thousand ceramic pellets. The A38 catalyst support is a cylinder of 3.42 mm in diameter and 3.46 mm in width, which gives a 3.90 mm volume-based particle diameter (i.e. the diameter of a sphere with the same volume as one of the pellets is 3.90 mm). As shown in Figure 1 a) and b), this pellet is discretised with 159 tetrahedra and the cylindrical container with 29,327 tetrahedra, for a total of approximately five hundred thousand elements for the whole model. In the numerical simulations the particles are modelled as rigid bodies with a density of 2.41 g/cm^3 and the interaction between each pellet is computed with a Coulomb coefficient of friction in the 0.6-0.9 range. The damping coefficient employed to represent the energy loss due to the impacts is in the 0.4-0.6 range.

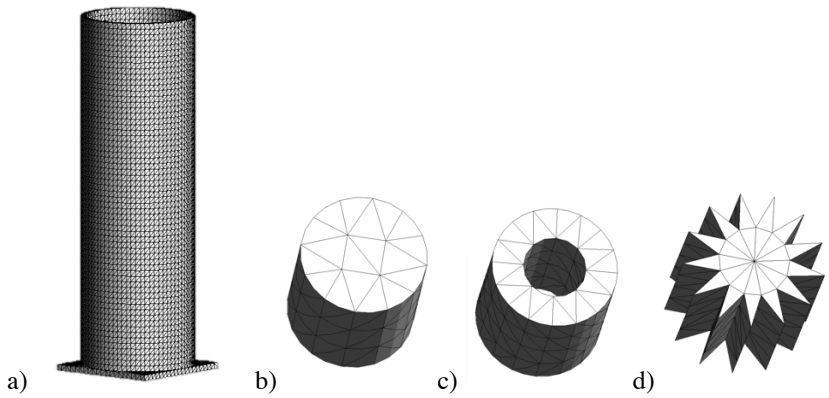

Fig. 1 Numerical discretisation of a) the cylindrical container, b) simple cylindrical pellet (A38), c) cylindrical pellet with one hole and d) tridecagram-shaped pellet

The final simulated packing structures for the three particle geometries are shown in Figure 2 a). Details of the simple cylinder and of the one-hole cylinder

packed structure are shown in Figures 2 b) and c) respectively. In Figure 2 d) a detail that captures the interlocking between the tridecagram-shaped pellets has been shown.

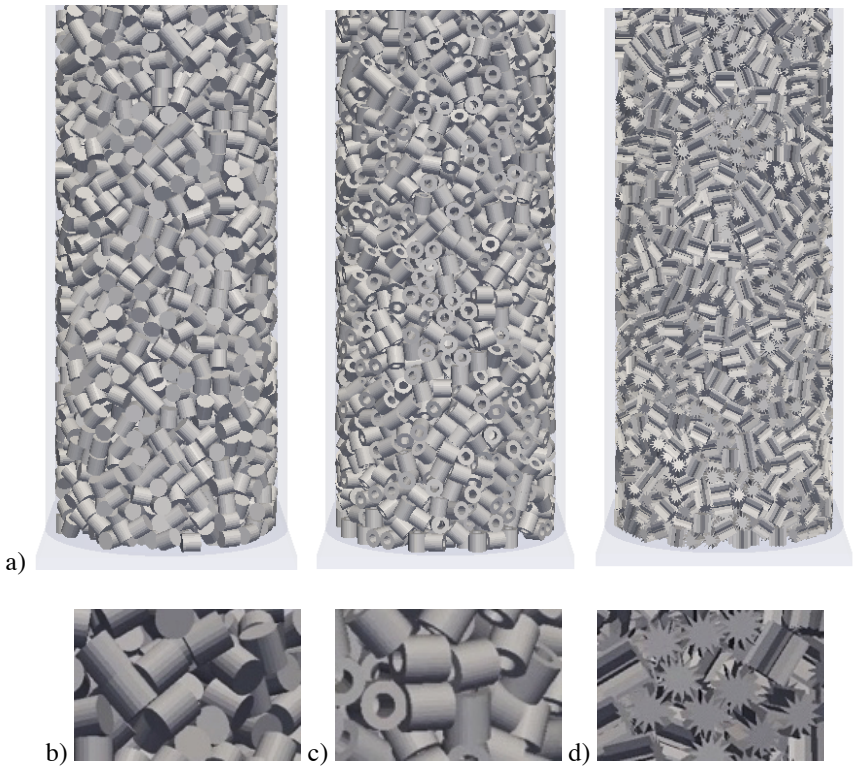

Fig. 2 a) Final simulated packing structures for the three particle geometries; details of the pack of b) A38 cylinders, c) one-hole cylinders and d) tridecagram-shaped pellets.

2.2 Post-processing

The numerical results are analysed with PORO, a post-processing tool that has been specifically developed to mimic the process employed to evaluate the axial and radial packing density profiles and the pellet orientation distribution from the X-Ray CT scans that has been employed in (2). In the following sections the post-processing algorithm will be described.

2.2.1 Axial and Radial Packing Density Profile

A regular grid is defined in the domain of the numerical results. A value of 1 is assigned to the centroid of the cells that are inside a tetrahedron of the solid mesh and 0 is assigned otherwise. For the sake of clarity in Figure 3 a) the cell dimension is similar to the dimension of the pellets. The real cell dimension is less than one tenth of the elements size, allowing a more precise discretisation of the packing density.

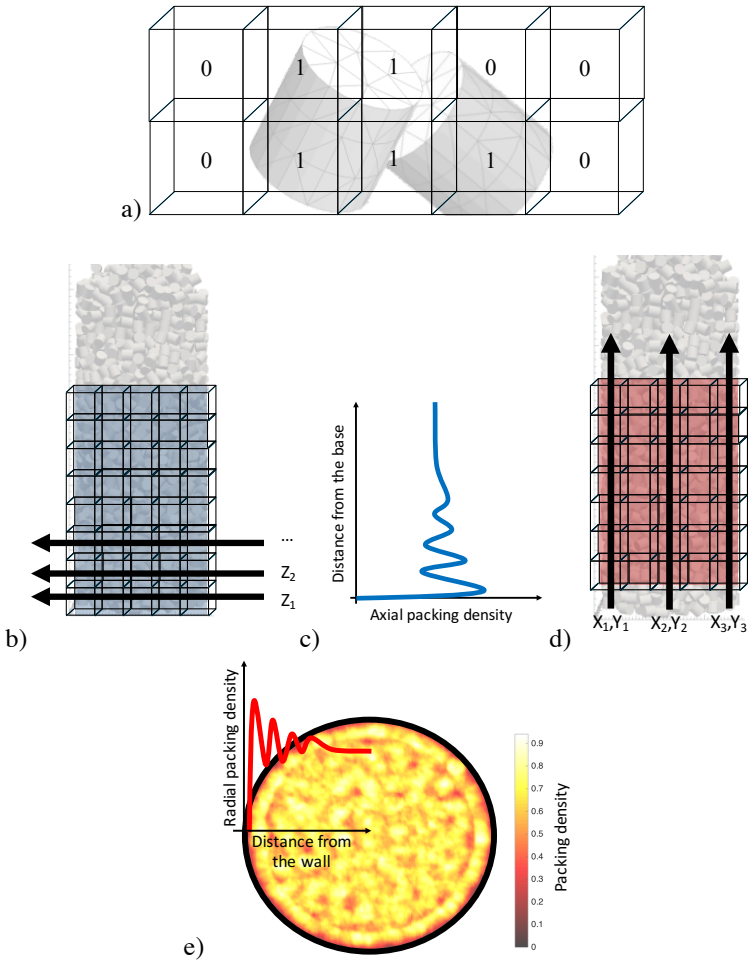

Fig. 3 a) Representation of the regular grid in the domain of the numerical results; b) averaging the values of cells along horizontal planes; c) axial packing density profile, d) averaging the values of cells along vertical columns; e) planar profile of the average packing density perpendicular to the axis of the container and radial packing density profile

The values of each cell is then averaged along horizontal planes to calculate the axial packing density profile, as shown in Figure 3 b) and c). The cells are then averaged along columns to obtain a planar profile of the average packing density perpendicular to the axis of the container as shown in Figure 3 d). The values on the plane are then averaged along concentric rings to calculate the radial packing density profile, as illustrated in Figure 3 e).

2.2.2 Vertical Orientation Distribution and Stereographic Projection

The coordinates of the axis of each pellet are calculated using the inertia tensor of the bodies and are exported at the end of the simulation to further characterise the packed structure. In particular, the angle between the axis of the catalyst support and the axis of the container (Figure 4 a)) is employed to generate statistics of the pellet orientations distributions that are then compared with the corresponding data form the X-Ray CT scans from (2).

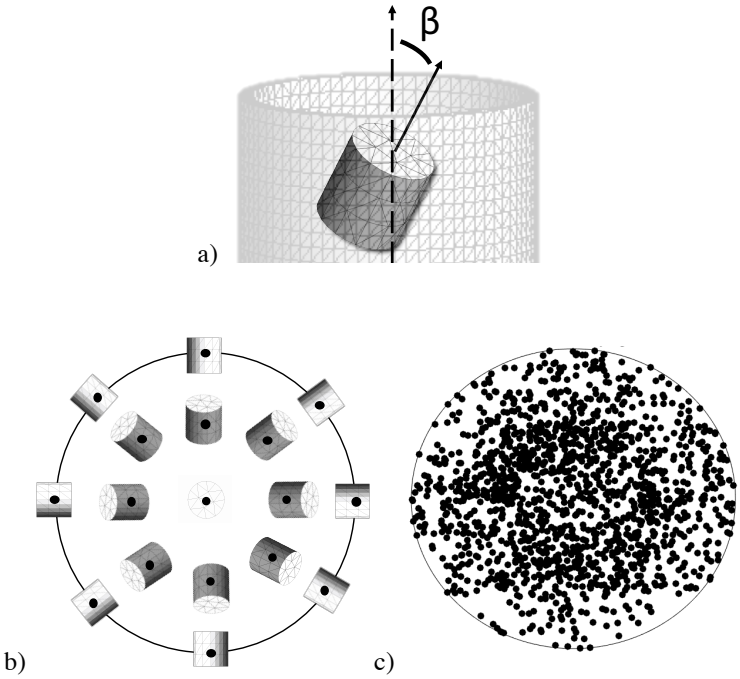

Fig. 4 a) Angle between the axis of the catalyst support and the axis of the container; b) plotted pellet orientations as they would appear from above the container; c) stereographic projection of the orientations of a cylindrical catalyst support packed structure

Lambert Equal Area lower hemispherical projections are generally used for presenting three-dimensional information on a two-dimensional plot. Stereographic projections are commonly employed in structural geology and geotechnical engineering applications (4), but they have been used also for concrete armour unit (5) and pharmaceutical tablets (6) orientation representation. In Figure 4 b) the equatorial reference frame represents the plane of the container base and the plotted pellet orientations are illustrated as they would appear from a top view. In Figure 4 c) the stereographic projection for the orientations of a simulated cylindrical catalyst support packed structure has been shown.

3 Results

The axial packing density profiles that have been calculated for the numerical simulations for the packing of the A38 catalyst supports have been plotted with the corresponding curve extrapolated from the X-Ray CT scans in Figure 5. Four FEMDEM simulations, corresponding to the four possible combinations of the extreme values for the friction and damping coefficients in the considered parameter space have been compared to the experimental results. Due to experimental constraints, the profile that has been reported in (2) represents the axial packing density from 3 to 17 particle diameters only. Because of this it has not been possible to compare the wall effects at the bottom of the container that have been captured by the FEMDEM simulations with the experimental curve. The numerical results are in agreement with the corresponding experimental results from the X-Ray CT scans. The fact that the simulated profiles present a higher amplitude and a frequency close to the particle size when compared to a relatively flat experimental profile suggests that the final packing structure in the numerical simulations is more ordered than the experimental pack. This could be an effect of possible differences in the loading conditions that have not been reported in (2), such as the dropping height, the number and the way the particles have been dropped inside the container, etc.

Similarly, the radial packing density profiles in Figure 6 show a good match between the numerical and the experimental results and confirm the stronger regularity in the simulated packing structures. The statistics of the pellet orientations for the angle between the axis of the catalyst support and the axis of the container that have been extrapolated from the X-Ray CT scans and from the corresponding numerical simulations of the A38 catalyst support pack are shown in Figure 7. Also in this case the numerical results are in agreement with the experimental distributions.

The stereographic projections representing the pellet orientations of the four numerical simulations are shown in Figure 8. Since the experimental statistics for the pellet axis azimuth angles have not been provided in (2), it has not been possible to make a comparison for this dataset.

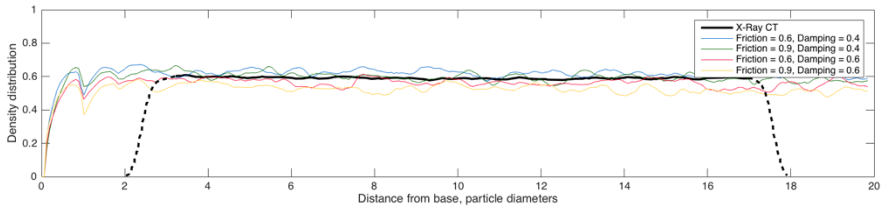

Fig. 5 Axial packing density distributions extrapolated from the X-Ray CT scans (in black), and from the numerical simulations of simple cylindrical catalysts with different values for friction and damping coefficients (in blue, green, red and yellow)

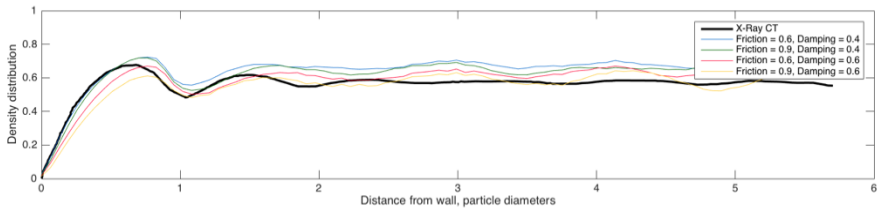

Fig. 6 Radial packing density distributions extrapolated from the X-Ray CT scans (in black), and from the numerical simulations of simple cylindrical catalysts with different values for friction and damping coefficients (in blue, green, red and yellow)

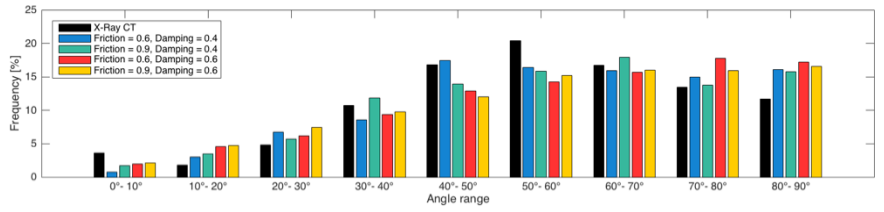

Fig. 7 Vertical orientation distributions extrapolated from the X-Ray CT scans (in black), and from the numerical simulations of simple cylindrical catalysts with different values for friction and damping coefficients (in blue, green, red and yellow)

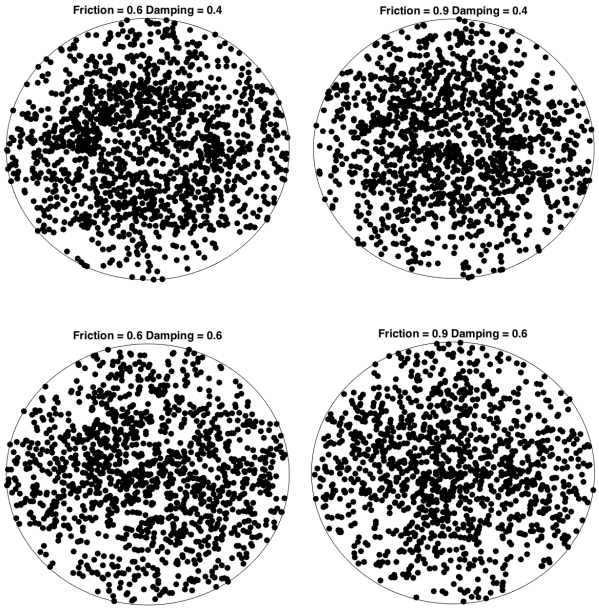

Fig. 8 Stereographic projections representing the pellet orientations of the numerical simulations with four combinations of friction and damping coefficients

4 Conclusions

Codes based on the combined Finite-Discrete Element Method (FEMDEM) are now widely used in research: more validation work needs to be undertaken to demonstrate their robustness and accuracy in simulating complex dynamic phenomena in multi-body systems for industrial applications. Some of the advantages of FEMDEM in modelling multi-body interactions for ceramic materials have been presented. These include the capability to represent the dynamic interactions between the catalyst supports during the loading phase and the potential to represent any complex-shaped body. Experimental and numerical results have been compared, confirming that a FEMDEM numerical simulation of packing of the A38 cylindrical catalyst supports in a cylindrical container matches the corresponding experimental results from X-Ray CT scans. These results give a first confirmation that a FEMDEM code can be used for the evaluation of performance-related properties of the pack. More confirmation might be obtained in the near future by studying the effects of the loading conditions on the final packing structure and by comparing the mechanical properties obtained from the simulations, such as the values of pressure on the container walls, with the results from actual packing experiments.

Acknowledgements

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