A Novel Physics-Based Algorithm for Modelling Random Packing Structures of Non-Spherical and Non-Convex Pellets

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Highlights

- An in-house Rigid Body Dynamics code 'RBDPac' was developed to investigate random packing of catalyst pellets.
- Mean and local void fractions have been obtained for random packings of spheres, solid cylinders and rasching rings with tube-to-pellet diameter ratio of 2 to 8.
- The influence of surface bounciness and friction of catalyst pellets on the structural properties were also investigated.
- This contribution, with the aid of validated data, discuses the merits of RBDPac in generating realistic random packing structures of non-spherical pellets.

1. Introduction

Fixed bed unit operations are extensively used in chemical and process industries with varieties of application such as tubular reactors to handle highly exothermic and endothermic catalytic reactions, thermal regenerators, adsorption towers and so on. The design of such systems is highly influenced by the structure of the packing matrix, which in turn is governed by the packing and container size and shape, the loading method, and the subsequent treatment of the bed. Today, the reliable and accurate design of such systems has become the topic of great importance. The inadequacy of macroscopic approaches, such as pseudo-homogenous models which neglect the role of bed structure, particularly in tubular fixed beds, is frequently addressed in the literature [1]. This has urged researchers to delve profoundly into the topological features of random packing structures such as spatial distribution of packings as well as their positions and orientations in a column, resulting in a multiplicity of in-house and *ad hoc* algorithms, see e.g. [2,3]. However, the majority of the prevailing efforts have dealt with the random packing of spheres, whilst application of catalyst pellets of non-spherical and often non-convex shapes, e.g. cylinders, raching rings, trilobes, etc., are becoming more and more popular because of their ability to enhance transport processes. Nonetheless, the amount of literature which addresses the structural properties of non-spherical packings are very scarce, e.g. [4,5]. This can be ascribed to the cumbersome and very complicated strategies to predict the trajectories of non-convex objects during the packing process, where the orientational freedom of such particles may not only be very problematic in terms of modelling, specifically when collision occurs, but also lead to exceptionally high computational expenses.
The main aim of this contribution is therefore to propose and scrutinize a state-based algorithm founded on Rigid Body Dynamics (RBD) to simulate the dynamics of random packing of even non-convex pellet shapes with high accuracy. Due to scarcity of available literature data on random packing of non-spherical pellets, validity of the simulation results was mostly inspected using the published data for spherical pellets.

2. Methods

RBD deals with the motion of rigid objects under the influence of external forces based on Newton's laws of motion as well as Lagrangian mechanics. Using this approach, the spatial behavior of a moving rigid object at time t is described by a state vector, X_i, which is comprised of the position of the center of mass, $x_i(t)$, a quaternion, $q_i(t)$, representing the rotation of the object in the word space, and linear and angular momenta, $P_i(t)$ and $L_i(t)$, respectively. The infrastructure of RBDPac is founded on resolving the rate of change or flow of state variables of packing materials over a time span, viz. the derivative of the state vector.

This boundary value problem is resolved using a midpoint method in an iterative mode, where the code takes initially both frictional and gravitational force fields into account. Upon collision (which is detected using a hard-body approach), the post collision mode is launched for colliding objects in which the collision phenomena are modelled using impulse theory. The flowchart of this code is illustrated in Figure 1.

3. Results and discussion

The results of packing simulations demonstrate satisfactory agreement with published data concerning global and local bed properties. For instance, the essential features, patterns and magnitude of the experimental data of radial void fraction distribution are well-reproduced (see Figs. 2 and 3). Furthermore, the postprocessing of results demonstrate a tremendous influence of surface properties of catalyst pellets on the simulated structures, as lower values of surface friction and higher magnitudes of restitution coefficient lead to denser packing structures.

4. Conclusions

This contribution, with the aid of validated data, substantiates the merits of the proposed RBDPac in replicating bulk and local properties of realistic packing structures of even non-convex pellet shapes, the subject, which has not been thoroughly addressed so far due to the complexities inherent in orientational freedom of such non-spherical pellets.

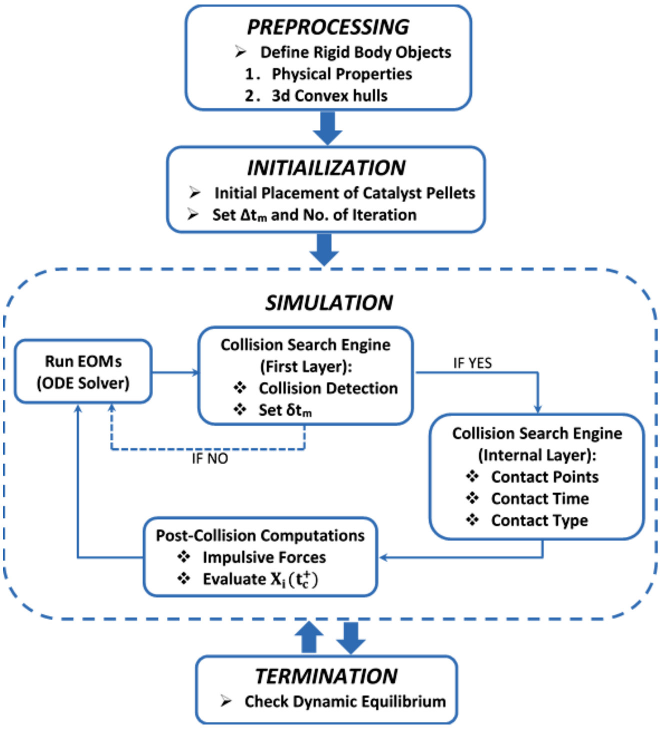

Figure 1. RBDPac algorithm flowchart.

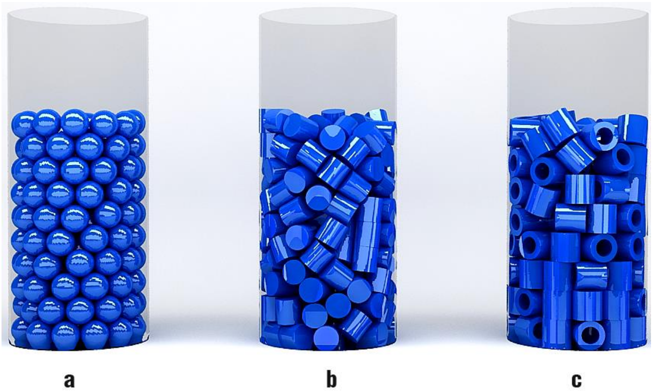

Figure 2. RBD-simulated structures of (a) spheres, (b) equilateral solid cylinders and (c) rasching rings, with $d_t/d_{pv} = 5$.

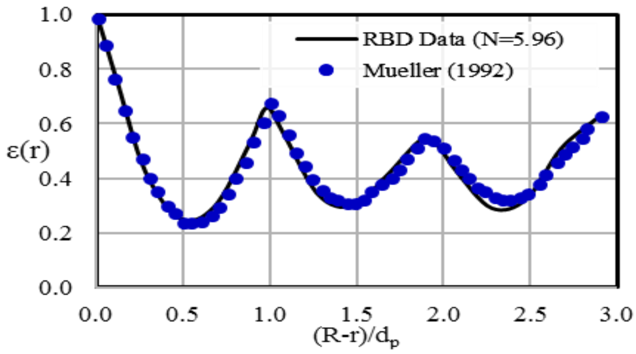

Figure 3. Radial void fraction profile for packing of spheres with $N = d_t/d_{pv} = 5.96$.

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Keywords

Fixed bed Structures, Random Packing Algorithm, Radial Void Fraction Distribution, Non-spherical Pellets, Non-convex Pellets.