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Validation of a novel open-source work-flow for the simulation of packed-bed reactors

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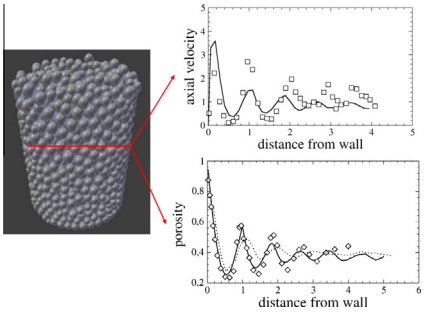
HIGHLIGHTS

- A novel open-source work-flow for the simulation of randomly packed-bed reactors is presented.
- Packing generation is performed with the open-source computer graphics code Blender.
- Fluid flow in the bed is simulated with the open-source CFD code OpenFOAM.
- The simulated packed-bed features are in line with experimental observations.
- Results prove that the work-flow is a cost and time efficient platform.

GRAPHICAL ABSTRACT



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ABSTRACT

The simulation of flow and transport in packed-bed (catalytic and non-catalytic) reactors is of paramount importance in the chemical industry. Different tools have been developed in the last decades for generating particle packings, such as the Discrete Element Method (DEM), whereas Computational Fluid Dynamics (CFD) is generally employed for simulating fluid flow and scalar dispersion. This work-flow presents the main drawbacks of being computationally expensive, as most packing generation algorithms deal with non-convex objects, such as trilobes, with cumbersome strategies, and of making use of in-house or commercial codes, that are either difficult to access or costly. In this paper a novel open-source and easily accessible work-flow based on Blender, a rigid-body simulation tool developed for computer graphics applications, and OpenFOAM a very well-known CFD code, is presented. The approach, which presents the main advantage of being computationally fast, is validated by comparison with experimental data for global bulk porosity, particle orientation, local porosity and velocity distributions, and pressure drop. To our knowledge this is the very first application of Blender for the simulation of packed-bed reactors.

1. Introduction

In chemical engineering many processes involve packed-bed (mainly catalytic) reactors and as such the study of momentum, heat and mass transport inside these systems is of great interest. Their investigation is generally performed by using both experimental and modeling techniques. The development of mathematical models, as in other areas of chemical engineering, is particularly interesting because it allows to collect more information and gain more insight. Different levels of resolution exist. In pseudo-homogeneous models the bed is treated as a single-phase

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system characterized by one single set of variables (i.e. temperature, concentration, etc.). In pseudo-heterogeneous models two distinct phases (e.g. the fixed bed and the moving fluid) are considered, but they are smeared out interpenetrating phases. In particle-resolved models the interface between the solid particles constituting the bed and the surrounding fluids is fully described, by using complex information concerning the relative positions of the particles. This last class of models is particularly interesting because it allows to investigate the relationship between (catalytic) particle properties (i.e. shape and size distribution) and packing features [1–4]. Moreover, after validation with experiments the working model can be efficiently used to design, scale up and optimize such systems, without resorting to costly and time-consuming experimental campaigns [5–9]. An additional advantage of developing mathematical models in this field, is that the mathematical model can be used to identify numerous features that characterize the fixed-bed, or packing, mainly related to local transport properties, that might, under some operating conditions, be hard to determine experimentally [10,11] .

A mathematical model for packed-bed reactors is mainly constituted by two modules: one that generates the geometry of the packing and one that simulates fluid flow. Usually the second task is performed by running Computational Fluid Dynamics (CFD) simulations [12–16], whereas for the first task two strategies can be used. The first lies on using actual experimental data, be it via Scanning Electron Microscope (SEM) imaging of the catalytic particles [17], micro-computer tomography scans of a portion of the packed-bed loading [18–20], or other such methods. While these procedures have a merit in the precision with which the description of the medium at the scale of the voids between the particles is obtained, they suffer from a great difficulty in the post-processing of these scans, in order to extract a suitable mesh for the CFD code. The second possibility, is to rely on an *in-silico* algorithmic reconstruction of a geometric model, which faithfully represents the real system in its most important features: the first advantage is the extremely lower cost of such an approach with respect to using the more sophisticated experimental techniques mentioned, coupled with the easiness of generating and testing a very high number of loading realizations, with varying particle shapes and particle size distributions. Obviously, great care must be given as to ensure that the reconstructed model is accurate both as a purely geometrical description and, perhaps more importantly, in showing the same fluid dynamic behavior of the real system under investigation.

The in-silico algorithmic reconstruction is often performed by using the Discrete Element Methods (DEM) [21–26] that present the main disadvantages of being computationally expensive, because of the accuracy with which fluid-particle interactions, negligible during packing generation, are described and being very often limited to the treatment of simple convex particles (i.e. spheres), whilst more realistic particle shapes (i.e. cylinders and trilobes) can be treated only with cumbersome strategies. This is particularly important because these exotic shapes, such as trilobes, are becoming more and more popular [27–40]. Other interesting alternatives are based on the use of Monte Carlo methods [41–43] that solve some of the above mentioned issues.

The objective of this work is therefore to introduce, test and validate an innovative approach for packing generation, alternative to DEM, still based on the classical ballistic theory of rigid-body simulations, but implemented in the very fast and computationally efficient computer graphics code `Blender` [44]. The main advantages of `Blender`, in comparison with alternative approaches, are: (1) the capability of dealing with particles of non-convex shapes, such as trilobes, very much used in catalytic reactors, (2) its being easy to use and open-source, therefore easily accessible, and (3) its being very fast. `Blender` has been in fact developed in the computer graphics industry where much effort has been directed towards time efficiency. The geometry in this way generated is than used to build a computational mesh and run CFD simulations in the `OpenFOAM` environment [45]. It is indeed interesting to observe that the developed work-flow, from geometry and mesh generation, to CFD simulation and post-processing totally relies on free open-source codes.

Since to our knowledge, this is the first application of the proposed open-source work-flow to the simulation of packed-bed reactors, a full validation is required. Therefore the capability of the tools to build realistic packings for three different catalyst particle shapes, namely spheres, cylinders and trilobes, is assessed, by comparing our predictions with experimentally measured packing bulk porosities, local radial porosity profiles and particle orientation distributions in cylindrical vessels. Subsequently, for each catalyst shape, the influence of some features of the particle size distribution on the resulting packing bulk porosity is analyzed. Also, a great deal of attention is paid to the meshing process. Meshes with different levels of refinement are tested and results concerning the evaluation of the critical cell size necessary to obtain both a good discretization of the particle surface and a precise description of the contact points between them, are discussed. CFD simulations are eventually performed on these systems by solving the continuity and Navier–Stokes equations and predictions regarding local radial velocity profiles and global pressure drops in the bed are validated by comparison with experimental data and empirical correlations. The final results prove that the proposed open-source work-flow is capable of simulating packed-bed reactors with very high accuracy and low computational costs.

2. Governing equations and theoretical background

`Blender` solves the Newton's equations of motion for a system constituted by N particles or bodies of arbitrary shape. It does that by availing itself of the Bullet Physics Library (BPL), which is a large collection of codes used to manage the dynamics of rigid-bodies and, most importantly, to detect and calculate the outcome of the collisions between these bodies. This library provides for a number of iterative methods combining accuracy, speed and robustness, enabling for the simulations of a very large number of elements, as it will be shown further on; moreover, a clear advantage of using this code with respect to many other algorithms used to recreate granular media models, lies in the possibility to manage any particle shape, even complex non-convex ones. An additional advantage lies with the fact that `Blender` does not consider the flow of the fluid in-between particles; being generally this fluid air, its presence has very little influence during the packing process. This makes the use of `Blender` more interesting, from the computational point of view, with respect to other similar codes, that instead do account for these effects (i.e. DEM). Details on the BPL can be found in the literature [46].

Once the geometry is generated, it is discretized and meshed within the `OpenFOAM` environment, which is an open-source finite-volume CFD code. The equations solved concern with the momentum and mass balance at the scale of the interstitial volumes left between the particles. For a fluid of constant density and viscosity, these are the well known Navier–Stokes and continuity equations; for a quick summary of these interstitial-scale equations, and their relationship with macro-scale equations, we remand to our previous work [47]. Here we limit the discussion to the macro-scale equations used for validation in this work.

From the macro-scale point of view, the pressure drop per unit length, $\Delta P/L$, in packed-bed reactors is calculated by using Ergun's law: