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Hydrodynamics of a packed bed of non-spherical polydisperse particles: A fully virtual approach validated by experiments

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HIGHLIGHTS

- Non-spherical polydisperse particles are measured using a caliper.
- A granular packed-bed is generated using DEM code.
- The flow inside of the bed is computed using CFD.
- Numerical predictions are only 16.0% from experimental data.
- The numerical workflow can explore parameter ranges unaccessible to the experiment.

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ABSTRACT

This work presents a numerical workflow to generate a virtual packed bed made of non-spherical polydisperse particles, and subsequently predict its permeability. Wood chips were taken as an illustration. First, chips are sized before being recreated numerically. Then, using LMGC90, a DEM code, a packed bed made of those chips was generated. Once bed internal had been sampled, CFD tools belonging to the OpenFOAM library were used to mesh the geometry (*snappyHexMesh*) and compute fluid motion (*simpleFoam*). Finally, using numerical results, the bed permeability was computed in both Stokes and inertial regimes - turbulence being described by Launder-Reece-Rodi model. In parallel, experimental measurements of the permeability of a packed bed, made of the exact same wood chips, was carried out. These experiments were used as a reference to challenge numerical results. The permeability value delivered by the workflow is 16.0% higher than the experimental value. This value has to be compared with Kozeny-Carman equation estimation which overestimates bed permeability by 115%. Going one step further, this framework was successfully used to compute inertial effects constant of the Forshheimer equation for our packed bed. Throughout this article, a special care has been taken in explaining and evaluating the impact of all the key parameters, namely, number of particles that have to be sized, mesh refinement level, numerical domain dimensions. This workflow opens the door to numerical estimation of bed tortuosity, dispersion coefficients, volumetric heat exchange coefficients, and much more, using the particle size distribution as unique input data.

1. Introduction

Nowadays, chemical engineering heavy relies on packed bed reactors. Most of the time, these beds are made of particles poured into a container which is then crossed by a reacting flow [1–4]. It is widely admitted that the hydrodymic properties - permeability, tortuosity, dispersion coefficients, …- of such devices are key to properly operate them [5–10]. Yet, they can be quite hard determine. Among them, permeability is of key importance as it directly influences the pressure drop across the bed, hence the pumping cost.

Three different approaches are available the determine this parameter. The first one is to use correlations coming from the literature such as Ergun [11] or Kozeny-Carman expression [12]. These semi-empirical correlations are widespread. They were derived, most of the time for packed bed made of monodisperse spheres. Even though, they can present refinements taking into account media made of non-spherical particles, polydispersed media and inertial effects, they usually only yield an estimation of the permeability.

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Nomenclature

Latin symbols

C	inertial constant, –
d	diameter, m
$\vec{f}$	body forces, N
$\vec{g}$	acceleration due to gravity, m^2/s
h	height, m
M	molar mass, g/mol
$\vec{n}$	normal vector, –
P	relative pressure, Pa
Q	volumetric flow rate, m^3/s
S	surface, m^2
$\vec{u}$	macroscopic velocity, m/s
V	volume, m^3

Greek symbols

α	Ergun equation Stokes regime constant, –
β	Ergun equation inertial regime constant, –
Δ	difference operator, –
ϵ	porosity, –
κ	permeability, m^2
μ	dynamic viscosity, Pa.s
ρ	density, kg/m^3
$\overline{\overline{\Sigma}}$	stress tensor, Pa
σ	surface tension, N/m
Ψ	sphericity, –

Subscripts

bed	bed
eq	equivalent
in	inlet
mesh	mesh
out	outlet
ref	reference
w–w	wood over wood
w–pvc	wood over PVC

Other symbols

∇	nabla operator
$\lvert\vec{a}\rvert$	norm
$\bar{a}$	arithmetic average
$\overline{\overline{A}}$	tensor

The second method consists in experimentally measuring the permeability value. The first experiments were carried out by Darcy [13] (Eq. (1)) who introduced the concept of permeability for porous media.

$$\frac{Q}{S} = \frac{\kappa}{\mu}\frac{\Delta P}{h} \quad (1)$$

This equation balances the most important parameters of the problem at stake. As fluid flows through a porous medium, it flows all the more rapidly that the pressure gradient is high, the medium is permeable and the fluid is close to being inviscid. Today, permeability measurements are quite common in the literature [14–18]. Usually, they consist in measuring, in steady state, a pressure drop over a bed crossed by a fluid of known viscosity under a well controlled flow rate (Eq. (2)).

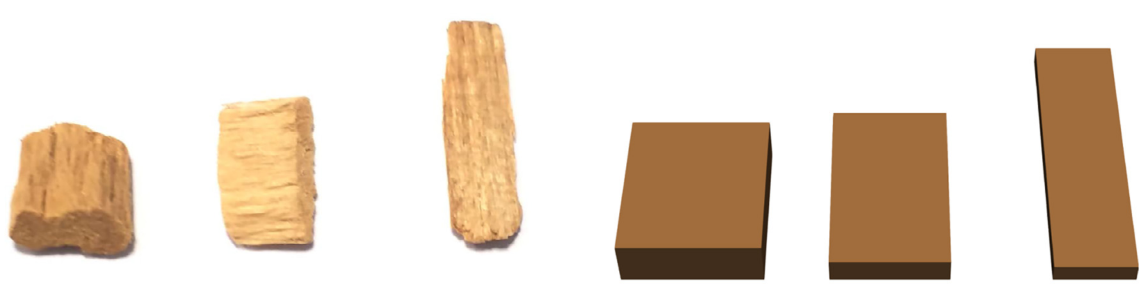
$$\kappa = \frac{Q\mu h}{S(P_{in}-P_{out})} \quad (2)$$

Yet, these measurements are not always easily conducted. Indeed, the flow has to reach steady state, which may take a tremendous amount of time for almost not permeable media, such as rocks [19] or tropical wood species [20]. The other extreme is very permeable media, that would induce only a minor pressure drop. In this case, the experimental apparatus has to be long enough so that a pressure drop can be precisely measured. Another technique is to use liquids instead of gases [21], as they have a higher viscosity. The drawback is that liquids are less convenient to use than gas namely because it is very difficult to ensure full saturation of the sample and to avoid degasing during measurement.

The last approach consists in using a numerical tool to assess for the physical properties. First, the medium is scanned [22]. Then, the void inside the solid matrix is meshed. Finally, using a Computational Fluid Dynamic - CFD - software, Navier-Stokes or only Stokes (when inertial effects are neglected, Eq. (3)) equations are computed in-between the solids in order to yield the fluid motion [23–25]. Then, the pressure drop across the numerical model is extracted and used to compute the permeability value. In addition, using a numerical approach, it is possible to obtain the different component of the permeability tensor [25]. From a more general perspective, this kind of numerical approach is spreading fast to different fields of science, such the design of heat exchanger [26–28] or static mixer [29,30].

$$Re = \frac{\rho\overline{d_{eq}}\lvert\vec{u}\rvert}{\mu} \lesssim 1 \quad (3)$$

The two last approaches are the most reliable, yet they require time and high quality materials: a permeability measurement apparatus for the experimental one, a 3D scanner for the last one. Furthermore, the fully digital approach suffers a drawback compared the experimental



(a) (b)

Fig. 1. Example of actual wood chips (a) and their numerical equivalents (b).