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Flow modelling through a packing of real particles

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ABSTRACT: The control of percolation in porous media is fundamental in geotechnical engineering and the assessment of its behaviour is predominantly performed by simple flow laws. In these constitutive models, where the medium is considered continuous, the variables obtained represent the average macroscopic behaviour of the flow in the porous medium and may be sufficient for determining and designing some practical problems in conventional engineering projects. However, the local variables in the voids can reach much different values from the average flow results on macroscopic scale modelling. These local levels can generate significant pressure drops and percolation forces that may cause engineering issues that the macroscopic models cannot predict. In this sense, this paper proposes the assessment of the flow behaviour through a packing of real particles by using a mixed numerical method methodology (DEM and VFM). The particles were characterized statistically by size and shape and packed randomly. The flow simulation was performed using a CFD software. With this model it is possible to evaluate the influence of the particles' morphology and assess the flow variables at the grain and pore-scale. The results were then compared with the well-known models of Ergun (1952) and Carman (1956).

Keywords: Flow modelling; Packing; Particles; Computation fluid dynamics; Microscale

1 INTRODUCTION

Fluid control in porous media is perhaps the most relevant problem in different geotechnical engineering projects and the analysis of flow behavior is predominantly performed by simple laws (eg Darcy's Law). In these models, where the porous medium is considered continuous, the variables obtained represent the average macroscopic behavior of the flow acting in a representative elementary volume. Macroscopic models may be sufficient for determining and designing some practical problems in conventional engineering projects. However, these average variables can be very different from the real values obtained in the flow that happens in the channels formed in the void matrix. A classic example of the insufficiency of the analysis by means of a macroscopic scale using the usual constitutive models is the prediction of erosion and particle dragging, since these levels of local variables can generate high percolation forces and cause entrainment of particles subjected to these efforts, when they overcome the forces resisting motion.

It is observed that, even after almost a century of flow through porous media scientific knowledge, the influence of flow at the microscopic level is still little known. Purely empirical criteria continue to be used in the vast majority of geotechnical projects that involve potential erosion prediciton, design of filters and drainage of permeable massifs.

Today, the development of modern particle characterization and virtual packing techniques that statistically represent real porous media serve as a basis for the development of grain and pore-scale flow models. These models can be initially structured from the fundamental equations of motion in fluids without the need to use macroscopic porous media flow models based on the representative elementary volume that encompasses solids and voids in a continuous medium. Allied to these techniques are the exponential advances in the processing capacity of computers, which enable the execution of solutions in extremely detailed and extensivemeshes for an accurate representation of the interface between solids and fluid in porous media. Additionally, it is possible to verify the validity of the macroscopic models when using microscale percolation analysis and how much the results of the local variables differ from the apparent mean results at the macroscopic scale.

In this work, a computational fluid dynamics (CFD) software was used, which operates with the finite volume method, in order to perform flow simulations through virtual packing of real characterized particles.

2 FLOW IN POROUS MEDIA

When it comes to porous media, fluid motion equations (Navier-Stokes Equations) refer to the continuous fluid that fills the voids in the porous media. However, the treatment of flow at grains scale using continuous fluid is not used in most engineering problems due to the inability to characterize in detail the geometry of the fluid-solids interface. In this regard, the continuum hypothesis enters as a more viable substitute. In this approach, the multiphase porous medium is replaced by a fictitious *continuum* and the variables are assigned using mean values for the elemental volume representative of the medium around a considered point. A problem arises related to how these average distributions are considered (Bear, 1972).

The systematization of flow through porous media began with Darcy in 1856 by means of experimental analysis, establishing a linear relationship between the specific volume flow and the hydraulic gradient. The hydraulic conductivity (k) is the proportionality constant of the model and depends on the properties of the fluid and the porous matrix. The fluid properties that affect hydraulic conductivity are density (γ) and viscosity (μ) and can be related to the intrinsic permeability of the porous medium by:

$$k = K\frac{\gamma}{\mu} \tag{1}$$

where K is the intrinsic permeability of the porous medium and k is the hydraulic conductivity.

Several formulas are described in the literature relating intrinsic permeability to various properties of the porous matrix. Some are purely empirical, others purely theoretical, derived from Darcy's law. The most known are: Kozeny (1927), Carman (1937, 1956) and Ergun (1952). As shown by Bear (1972), all these equations have the general formula:

$$K = f_1(s)f_2(n)d^2 \tag{2}$$

where $f_1(s)$ is a function that expresses the effect of grain (or pore) shape, $f_2(n)$ is a function that expresses the effect of porosity, and d is the effective (or average) diameter of the particles.

Although these equations are interesting as an evolution of Darcy's law, they can be considered unsatisfactory for understanding the behavior of the microscopic flow because they involve a high degree of simplification of the flow and of the real porous media. This occurs especially due to the need to choose ordered porous media to enable the theoretical and mathematical treatment, in contrast to real porous media, which are highly disordered (Bear, 1972).

The purpose of the analysis presented in this paper involves avoiding these classic models, simulating the flow on a microscale using the Navier-Stokes equations without geometric simplifications, seeking to evaluate the flow behavior through the porous media on a microscopic scale.

3 PORE-SCALE CFD SIMULATION

The methodology proposed for the work is given by the combination between the discrete element method (DEM) represented by the particle pack and the finite volume method (FVM) through computational fluid dynamics (CFD), which includes numerical methods using the continuum hypothesis for the fluids. The models were processed by a CFD software, with pre and post processing support.

3.1 Particle characterization and packing

The initial stage of modeling is carried out from the characterization of the material to be used. For the models presented in this paper the chosen material is coarse aggregate supplied by a quarry, located in the Federal District, Brazil. The aggregates are initially characterized by particle size and morphology. Then, image captures are performed with post processing in order to digitally obtain surface meshes for each individual particle (Figure 1). The morphology of the surface is defined by Fourier or Spherical Harmonic descriptors and through the repetition of the process on a sufficiently large number of particles, it is possible to obtain statistical distributions that define these parameters for the whole set of particles. From these distributions, a bank of virtual particles that statistically represent the real particles is created.

Packings are then generated through the selection of random particles within the bank, and tridimensionally bringing the particles closer to each other using algorithms such as those presented by Morfa et al. (2017) and Recarey et al. (2019). These packings are capable of statistically representing not only the grain size distribution of the chosen material, but also the shape of the particles itself.

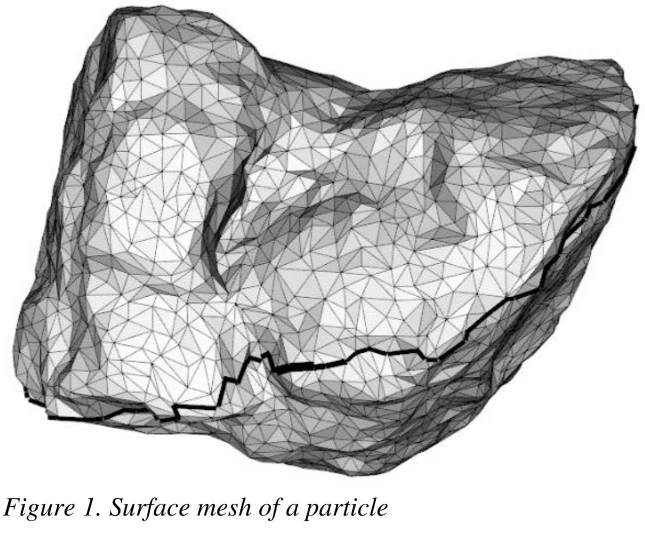

Figure 1. Surface mesh of a particle

3.2 Particle Pack Geometry

The packing used in the analyzes was adapted from the packing generated for a micromechanical analysis with binder material and fine aggregate. These materials were removed from the model, leaving only the coarse aggregates (Figure 2). Therefore, not all particles in the model have at least one contact with another particle.

Therefore, the packaging does not exactly represent a specimen made strictly with gravel, since not all particles have defined contacts, but by obtaining the porosity, the results can be evaluated without major problems.

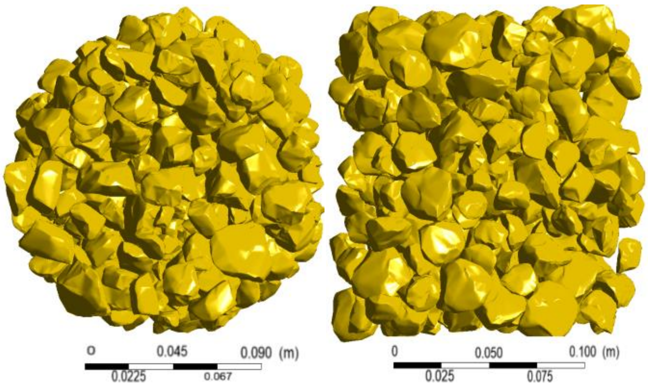

Figure 2 Pack of 450 particles

The particles themselves were constructed virtually with a surface mesh of 200 coordinate points for each particle in the model.The measurement of the porosity of the model was performed directly by a 3D CAD modeling software. The resulting porosity of the model was 0.62. Figure 3 shows the packing void matrix.

The particles have a nominal diameter between 9,5 and 19 mm. This packing is inserted inside a cylinder where a constant velocity inlet was applied at one end and zero pressure outlet at the other end, forcing the flow to percolate through the particle pack. The cylinder has an internal diameter of 16,8 cm.

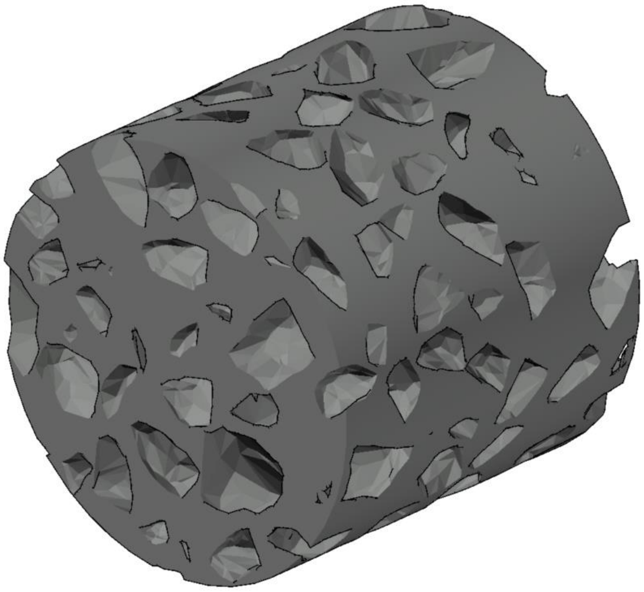

Figure 3. Void matrix

3.3 Flow modeling

The creation of the mesh goes through three main steps. The first is the creation of a *surface mesh* that triangulates the entire surface of the solids contained in the model. The second step is the definition of the boundary conditions and the creation of the region that will be filled by fluid. Finally, the last step is the creation of the three-dimensional volumetric mesh (*volume mesh*). This mesh is generated across the fluid region based on the previously initially generated surface mesh. One can consider or not the solids of the model for the triangulation. The elements used are polyhedral.

Interestingly, due to the size of the particles and the scale of the problem, the resulting mesh is quite large, with more than six million elements. The voids between particles can also be quite small compared to the average particle diameter, requiring even greater detail in these regions to obtain a high quality mesh.

After the elaboration of the mesh, the model parameters and boundary conditions must be detailed. For the model carried out, input boundary conditions such as constant velocity and output boundary condition as constant and zero pressure (atmospheric pressure) were used.

The modeling carried out is in a laminar regime, with a Reynolds number always reduced, so there is no need to use a turbulence model to solve the model. The fluid is water, considered incompressible for these stress levels, and the model is always fully saturated.

For the convergence control, the established limits are in terms of residuals of continuity and velocity in the three directions. Since the density and viscosity of the fluid are constant for the models, it is not necessary to introduce the energy conservation equation into the system.

3.4 Boundary conditions

Three different inlet conditions were established, all of them with a fixed velocity value and obtaining the pressure distribution as a consequence. The inlet velocities were v=0.01 m/s, v=0.001 m/s, and v=0.0001 m/s. This parametric analysis was carried out to evaluate the distribution of velocities and pressure in the fluid with different characteristics generated by the different inlet conditions.

The outlet was always maintained at a pressure equal to atmospheric pressure. Therefore, whenever the inlet velocity is increased, the pressure difference between the inlet and outlet is also increased.

The cylinder adopted as an external envelope is 75 cm long and the particle pack is positioned between 20 and 35 cm. Boundary conditions were established at the ends of the cylinder inlet and outlet to favor flow stabilization.

4 RESULTS

This section presents some results obtained from the models executed for flow through a pack of real particles. The results for the models presented in this section have not yet been experimentally validated. However, the results succeed to show the potentiality of the methodology presented for the characterization of poroscale flow.

From the computed results, it is possible to obtain the streamlines. These lines represent the flow paths from the entry in the model to the exit and can be used to extract various information, both geometric and simulation results. Figure 4 presents the *streamlines* obtained for the reference model.

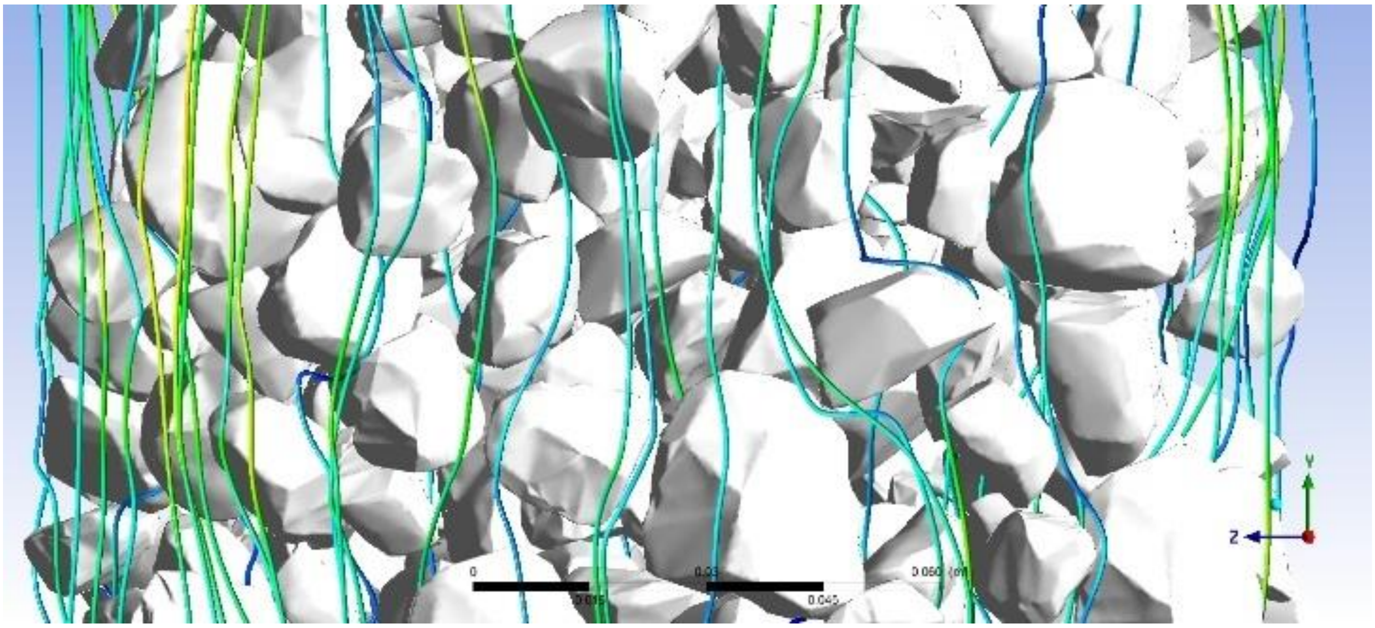

Figure 4. Streamlines obtained

A by-product of the result streamlines that can be obtained with post-processing is the tortuosity, which is defined by the ratio between the length of the fluid's path and the straight length of the particle pack. This variable is very relevant for the characterization of the void matrix and is used in established models such as Kozeny-Carman in Carman (1956) and several other derived models. Usually, tortuosity is always difficult to obtain and is estimated by means of approximations or empirical formulations as in Katagiri et al. (2017). In the methodology presented here, tortuosity is a product that can be extracted directly from de model, without any approximation. The results are shown in Table 1.

Table 1 Tortuosity calculated from the model flow lines

Tortuosity	
Average	1,133
Maximum	1,329
Minimum	1,022

Note that the tortuosity represents how much the path of the fluid through the void channels differ from the lenght of the pack and deppends on the porosity, the morphology of the particles and void channels. It represents a major influence on the pressure drop along the porous media.

Figure 5 shows the *u* velocity (left) and pressure (right) distribution graphs along all the streamlines mapped in the packing region (20-35 cm). Trendlines are also plotted on pressure graphs to assess the dispersion of pressure values from the mean.

With the graphs of the pressure distribution in Figure 5, it is possible to clearly see that the dispersion of the pressure value at each point in relation to the average is greater when the inlet velocity is increased and, consequently, the total pressure difference. On the other hand, the relation between the maximum local velocity and the entrance velocity (which is the same as Darcy's apparent velocity) is reduced when the pressure difference between the packing ends grows. Table 2 presents the summary of the main values obtained in the graphs presented.

Table 2. Summary of results

Inlet velocity (m/s)	**Maximum *u* velocity (mm/s)**	$\frac{v_r}{v_i}$	ΔP **(Pa)**	**R^2**
0.0001	0.897	8.97	3.61E-03	0.9611
0.001	7.22	7.22	4.79E-02	0.9549
0.01	49.1	4.91	1.37E+00	0.9026

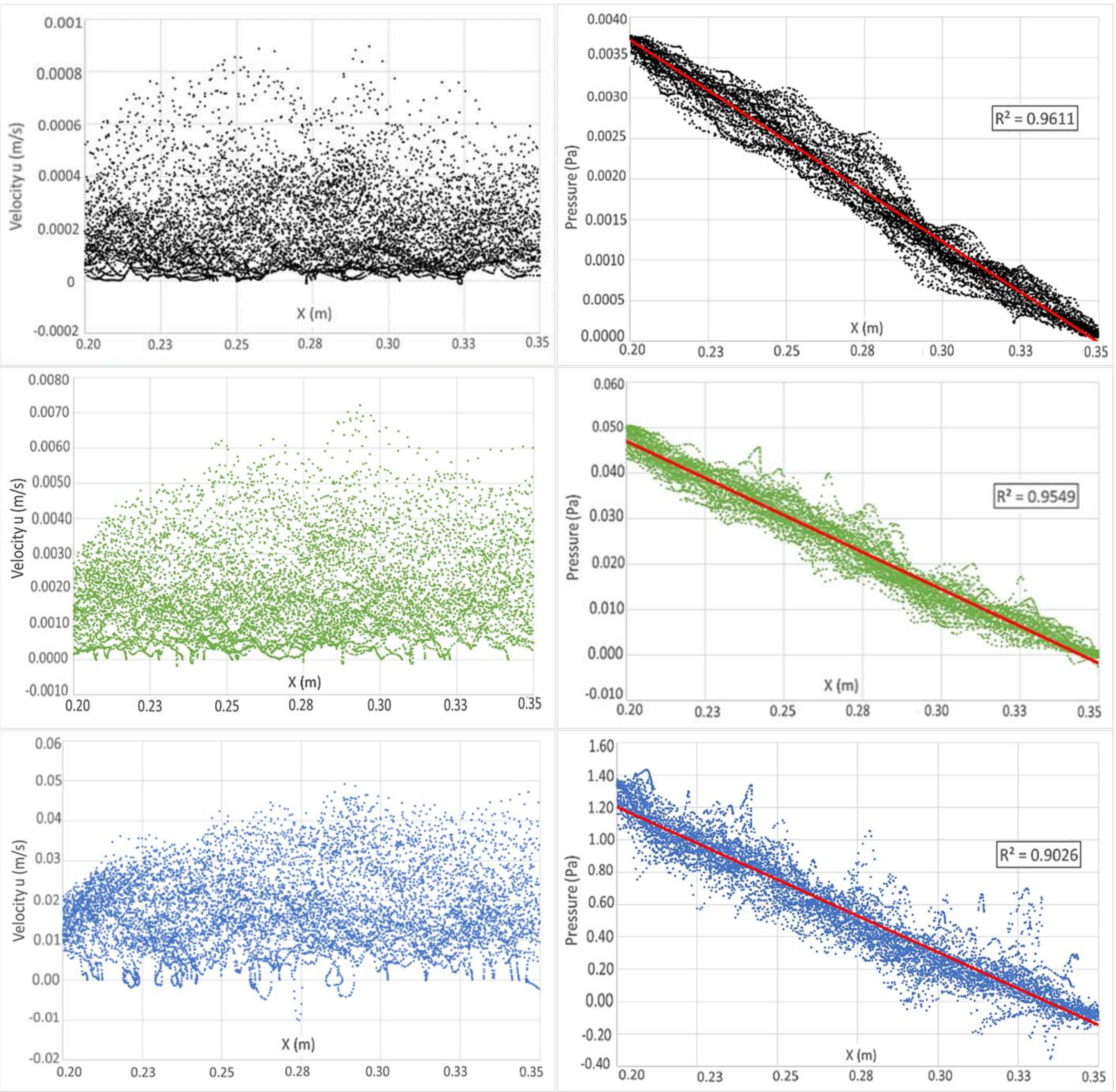

Figure 5. Results of velocity and pressure distribution along the packing

For comparative purposes, pressure drops estimated using the Kozeny-Carman equation on Carman (1956) and Ergun (1952) equations were obtained. It is known that there are numerous models derived from these other two, such as: Glover et al. (2006), Katagiri et al. (2017), Koch et al. (2012), Latief and Fauzi (2012), Ozahi et al. (2008), Ren et al. (2016). However, all these models use more or less the same parameters presented in the equations of Kozeny-Carman and Ergun and a universal macroscopic model has not yet been proposed that solves the difficulties in obtaining the input parameters and that does not involve excessive simplifications, both geometric and physical. Therefore, the results from the Kozeny-Carman‘s and Ergun‘s equations will be used as a refference point for the results obtained in the numerical models. Figure 6 presents the resuls and Table 3 presents the summary of the pressure drop estimations from the equations mentioned and the models‘ results. The axes in Figure 6 are on a logarithmic scale only to help the visualization.

It is possible to verify that the concordance of the results obtained with the models is greater the smaller the pressure drop and, consequently, the inlet velocity. For higher values of inlet velocity, the results obtained by the two equations are quite discrepant, reaching a difference of more than 6 times for an entry velocity of 0.01 m/s. The numeric model with this input velocity shows a pressure drop result that is not compatible with either of the two reference models.

It is essential to point out that the equations by Kozeny-Carman in Carman (1956) and Ergun (1952) were developed considering numerous simplifications, mainly geometric and using as input average data that is also difficult to estimate, such as the mean velocity in the mean pressure section of the Ergun formulation or the shape factor of the Kozeny-Carman (K-C) formulation.

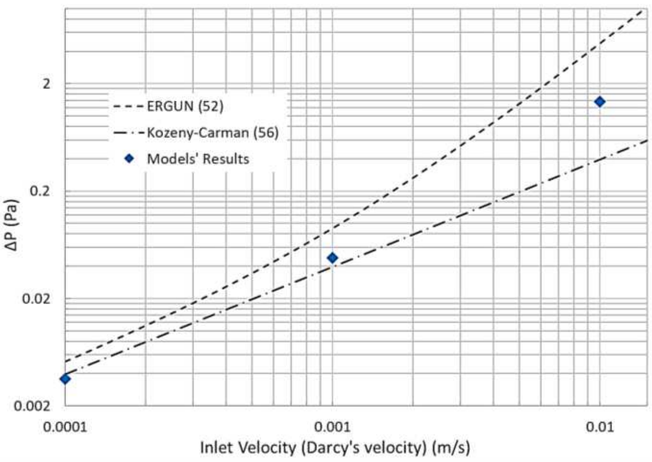

Figure 6. Modelled pressure drop results

Table 3. Results and Kozeny-Carman's and Ergun's models

Inlet velocity (m/s)	**ΔP (Pa)**	**ΔP - Ergun (1952) (Pa)**	**ΔP - Kozeny-Carman (1956) (Pa)**
0.0001	3.61E-03	5.39E-03	3.94E-03
0.001	4.79E-02	9.07E-02	3.94E-02
0.01	1.37E+00	2.38E+00	3.94E-01

5 CONCLUSIONS

The use of numerical models for assessing flow in packings of particles with real morphology is a powerful tool for understanding the flow through porous media. The union of discrete (particles) and continuous (fluid) numerical methods allows evaluating and verifying the validity of well-known models of flow in porous media and opens a door to understanding the macroscopic phenomenon using the poro-scale.

The results have shown that the local pressure and velocity can be quite different from the section average values. The greater the pressure drop in the packing of particles, the greater the local pressure values will differ from the section average.

Regarding the reference equations (K-C and Ergun), the results showed relative agreement with the models for low pressure drops in the particle pack. However, for higher input velocities (Darcy's velocity), the estimates of the reference models are very discrepant and do not adhere with the result of the numerical model.

It is known that the results will benefit from further experimental results, but the methodology already represents an alternative for solving significant limitations of the macroscopic models for flow in porous media.

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