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A DEM-CFD APPROACH TO PREDICT THE PRESSURE DROP THROUGH AN AIR-ROCKBED THERMAL STORAGE SYSTEM: PART 1

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Abstract

This paper, the first of two, explains the methods used to create an irregular packed rock bed with the DEM and how the developed geometric model can then be converted into the appropriate format, such that a method to predict the pressure drop over the bed, by means of a CFD analysis can be developed. It started by first investigating the degree to which the DEM input parameters affect the porosity of a bed with spherical particles and the results showed that only low internal friction coefficients have a significant effect. At the same time it was established that the porosity of a bed consisting out of irregular shaped particles cannot be obtained if only spherical particles are used in the models. However, when the particle shape and size distribution was improved by clumping several spheres together in order to model the non-spherical particles, the correct porosity could be obtained.

Key words: DEM, packed rock bed, input parameters, internal friction coefficient, porosity, angle of repose

1. Introduction

The increased necessity to obtain power from other sources than conventional fossil fuels has led to the growing interest in solar power. Not only is this technology improving, but large scale solar thermal power plants are being built in a number of countries around the world. Unfortunately there are countries, such as South Africa, which has some of the highest irradiation levels in the world, but is still not using it to its fullest potential. The reason for this might be the fact that solar power plants have high capital cost and require large areas of land. It is therefore crucial to investigate methods to reduce these factors and one such method is the SUNSPOT cycle (Stellenbosch UNiversity Solar POwer Thermodynamic cycle). The SUNSPOT cycle is a thermal power generating plant, which is being evaluated and developed by the Department of Mechanical and Mechatronic Engineering at the University of Stellenbosch. It was proposed by Professor Deltev Kröger in 2008, because it is an efficient and appropriate means of generating electricity in South Africa [1]. Research on the SUNSPOT cycle is being done by the Solar Thermal Energy Research Group (STERG) and one of the primary research areas is the rock bed thermal storage unit, especially with regard to the pressure drop over the bed.

Currently there are numerous analytical models available to predict the pressure drop over packed beds of which some of the most common are the representative unit cell model [5] as well as the equations of Ergun [6] and Singh [10]. However, the use of Computational Fluid Dynamics (CFD) to predict the pressure drop has become more and more popular in the past few years. In most of these studies, only small amounts of particles are usually modelled and they are packed in structured manners such that the models could accurately and easily be reconstructed in CFD. If one is therefore interested in applications where a large number of particles are randomly packed, such as in the thermal storage rock bed where it is impossible to directly measure the position of the rocks in order to create the CFD model, the Discrete Element Method (DEM) could be incorporated. This coupled DEM-CFD approach has been used by a number of researchers, but according to Chung [3], one crucial aspect which was not adequately addressed was how their DEM input parameters were selected or determined such that satisfactory quantitative predictions could be produced. In many cases the input parameters were assumed without the proper justification and often not even measured.

This paper will therefore address this issue by discussing a sensitivity analysis which was conducted in order to investigate the degree to which the input parameters would affect the porosity of a developed DEM model of a randomly packed bed with spherical particles. It then moves on to explain how a DEM model of a packed bed with non-spherical particles can be developed as well as how the model porosity would be affected by the input parameters. This is important, because Part 2 of this paper will focus on developing a method to generate a mesh on a bed with irregular shaped particles such that a CFD analysis can be performed in order to perform pressure drop predictions. Finally, because the DEM software used in this study has no means of exporting the developed geometric model into the appropriate format such that a CFD analysis can be conducted, a method to convert the geometric model into the appropriate format is discussed.

2. The Discrete Element Method

Currently most of the numerical methods that are based on continuum mechanics represent the discontinuity and inhomogeneous nature of geo-materials such as rocks and soils implicitly and are limited when large scale models in three dimensions are required. Fortunately an alternative to these methods is the DEM, which makes use of an assembly of independent elements to represent the material under consideration. By using independent elements the problem with implicitly representing the discontinuity and inhomogeneous nature of geo-material is eliminated because they are explicitly reproduced at the boundary of each individual element. However, DEM is mostly suited for the modelling of granular material, but it can still be used for geo-materials. This is achieved by simply using cohesive forces to bond groups of discrete elements together in order to resemble the desired geo-material [4].

3. Sensitivity Analysis

In order to successfully simulate a packed rock bed with the DEM, the following input parameters need to be defined: the density of the particles, the internal friction coefficient (the friction coefficient between contacting particles), the particle-wall friction coefficient (the friction coefficient between particles and system boundaries), the damping characteristics (in the form of local damping coefficients as well as normal and shear critical viscous damping ratios), the particle-particle contact stiffness, as well as particle-wall contact stiffness and finally the particle shape and size distribution [9]. The sensitivity analysis therefore worked on the basis of varying one of the input parameters in the numerical models, while keeping the rest constant, so as to compare the resulting bulk characteristics to those of an actual experimental bed. These bulk characteristics include the bulk density, the bulk stiffness, the internal friction angle, the porosity and the angle of repose. However, due to the fact that the focus of the papers criticized by Chung [3] was to predict the pressure drop over a packed rock bed by using a DEM-CFD approach, the focus of this study was purely on the was on the porosity and the angle of repose. This is acceptable, since from a DEM point of view, the pressure drop is primarily influenced by the packing structure of the bed (particle shape and size distribution, packing arrangement and void spaces) and the angle of repose as well as the porosity will also give a good indication that the packing structure is indeed accurate [11].

3.1 Experimental work

The purpose of the experimental work was to obtain all the required input parameters as well as the required bulk parameters, but due to unavailability of certain sophisticated test equipment only some of the input parameters could be obtained experimentally. The rest had to be obtained from literature. Nevertheless, this did not pose any problems since the most important values, the porosity and angle of repose, could be obtained experimentally, while the rest only required estimates. The first step was to select an appropriate bed size on which the numerical work would be based. A cylindrical steel container with a diameter of 0.59 m and a height of 0.33 m was selected in that together with the bulk material selected for this study, it would provide a bed with a high aspect ratio. This meant that the wall effect is reduced and the numerical models would not have to simulate large amounts of particles, which directly influences the computational time.

The bulk material under consideration is coarse crushed aggregate with an averaged equivalent diameter of about 30 mm (based on the particle volume) and it was obtained from the Portland quarry located in the Western Cape of South Africa. It was selected, because it would also be used for additional rock bed thermal storage experiments being conducted by other researchers at the Department of Mechanical and Mechatronic Engineering of the University of Stellenbosch. Before the bed was filled several particles were collected in order to determine the particle density, ρ_p. This was achieved by simply dividing the mass of the particles by their volumes, which gave an average particle density of 2610 kg/m^3. Once the particle density was obtained the bed was carefully filled and then leveled. During this process the mass of the particles going into the container was recorded such that the bulk density, ρ_b, could be obtained by simply dividing the bulk material mass by the bulk volume. This was done for several bulk samples to obtain an average bulk density of 1339 kg/m^3. One should not mistake the particle density with the bulk density in that the two differ in the sense that the bulk density includes the voids between the particles in the bulk sample, whereas this is not true for the particle density. Both densities are however required in order to calculate the voids ratio, e. The voids ratio is defined as the ratio between the total void volume and the total particle solid volume. The porosity, ŋ, can then be defined in terms of the voids ratio as follows [8]:

$$ŋ = \mathbf{100}\left(\frac{\mathbf{e}}{\mathbf{e+1}}\right) = \mathbf{100}\left(\frac{\frac{\rho_p}{\rho_b}-\mathbf{1}}{\frac{\rho_p}{\rho_b}+\mathbf{1}}\right)$$

The average porosity was estimated to be 0.487 using this procedure. Once the porosity was determined the angle of repose, α, could be measured. This bulk parameter can be obtained by allowing the bulk material sample to form a pile and then to measure the inclination of the free surface of the pile to the horizontal. This is a very important bulk parameter, because it depends largely on the particle shape and size distribution of the material as well as the friction between the particles. The experiment was conducted by filling a bottomless plastic bucket, resting on a plywood board, with the bulk material. The bucket was then lifted manually and very slowly so as to form a pile as can be seen in Figure 1.

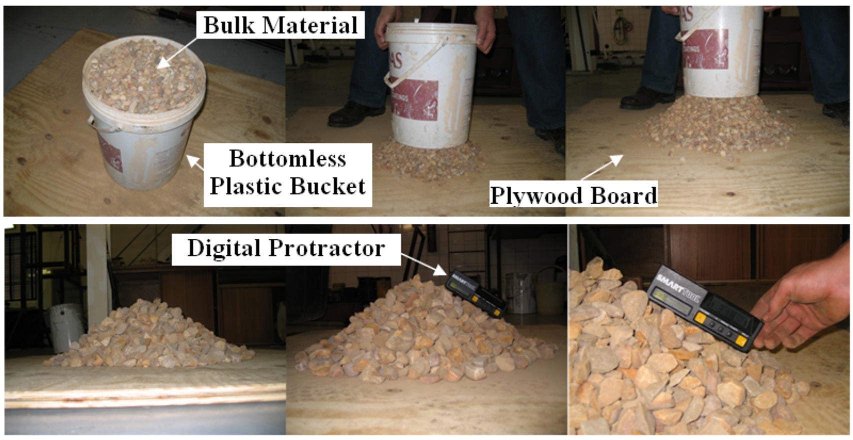

Figure 1: Angle of repose test

A number of surface angles were then measured, using a digital protractor and the experiment was repeated several times to obtain an average angle of repose of 32.5°. The angle of repose experiment also has the advantage that a rough estimation of one of the micro parameters, the internal friction coefficient, μ_{pp}, can be obtained by means of the following:

$$\mu_{pp} = \tan \square$$

This approach gave an internal friction coefficient of 0.71. On the other hand, the rest of the input parameters, which could not be obtained with the proper experiments, were taken from the literature such that the numerical simulations for the sensitivity analysis could be performed.

The initial input parameters that were used for this study can therefore be summarized as follow:

- An equivalent particle diameter of 30 mm
- A particle density of 2610 kg/m^3
- An internal friction coefficient of 0.71
- A particle-wall friction coefficient of 0.71 (taken as similar to the particle-particle friction coefficient)
- A damping ratio of 0.8 for the normal and shear viscous coefficients
- A local non-viscous coefficient of 0.0
- A contact stiffness of 1.72 x 10^6 MN/m for the particle-particle contacts and 1.0 x 10^{10} MN/m for the particle-wall contacts

3.2 Numerical work

The numerical simulations were performed with the commercially available DEM package, PFC^{3D}, which was developed by the Itasca consulting group in Minneapolis [9]. The common methodology is to start by first creating the system boundaries or in this case the walls resembling the cylindrical container used to determine the bed porosity as well as the walls of the bottomless plastic bucket for the angle of repose test. Once the system boundaries are in place, they are filled with a predetermined number of particles (in DEM these particles are simply spheres) and allowed to settle. This filling process is usually achieved by simply generating the particles in random positions above the container to be filled and then allowing the particles to fall under gravity. This is commonly known as the rainfall method (Figure 2). However, this method was not selected, because it did not accurately resemble the filling procedure used in the experiment, where the rocks were poured into the container from a bucket at a relatively low height. This was due to the fact that with the rainfall method a large percentage of the particles drop from such heights, that they produce a bed which is more compact than the actual experimental. It was therefore decided to modify the rainfall method such that the particles first drop and then settle onto plates just above the container after which the plates can slowly be removed such that the particles can be dropped into the container from a much lower height (Figure 2). This was verified by simulating the two methods with the initial input parameters and the results showed that the rainfall method did indeed lead to a lower porosity (more compact bed) than the modified method.

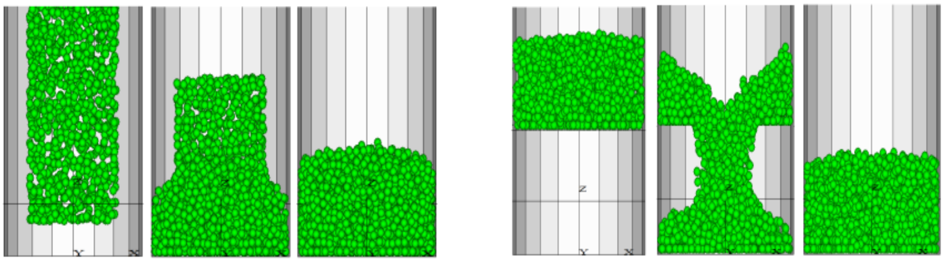

Figure 2: Filling a container with the rainfall method (left side) and with the modified method (right side)

The next step was to perform several simulations where each input parameter was changed three to five times, while the rest remained constant. The numerical porosity would then be determined for each simulated condition such that it can be compared to the experimental porosity. The results showed that the input parameters, which would most likely have an influence on the bed porosity, namely the internal friction coefficient, the particle-particle contact stiffness and the particle density had no significant effect. The only noticeable influence was at very low internal friction coefficients (Figure 3), which can be explained by the fact that at those conditions the spheres are practically frictionless and therefore form a very dense packing structure.

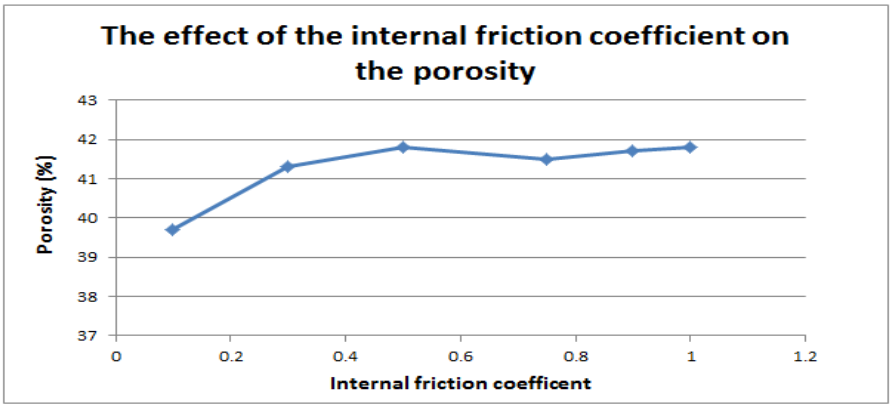

Figure 3: The effect of the internal friction coefficient on the porosity for a bed with spherical particles

Similar results were obtained for the particle-wall contact stiffness as well as the particle-wall friction coefficient, but this was expected due to the bed's high aspect ratio, which decreases the wall effect tremendously. The damping characteristics also had a very little effect on the porosity in that they usually have a much bigger influence on dynamic systems rather than static ones. It can therefore be concluded that even though Chung [3] was right in criticizing many authors whom implemented a coupled DEM-CFD approached for pressure drop predictions, to not have adequately justified their DEM input parameters, their results can still be regarded as reliable. This is because even if some of their input parameters were chosen incorrectly, the numerical porosity and therefore the pressure drop over the beds would not have been greatly affected. Still, care should be taken when particles with very low internal friction coefficients are modelled in that they could have a significant effect on the porosity. Similarly, if beds with relatively low aspect ratios are modelled the particle-wall friction coefficient as well as the particle-wall contact stiffness could have an influence on the porosity.

Another important aspect to consider is that the DEM models had and average porosity of 0.415, which corresponds to an error of 14.8 %, when compared to the experimental porosity of 0.487. This is due to an inaccurately specified particle shape and size distribution and can be proven by simulating the angle of repose experiment. This was done and the results showed that even when the internal friction coefficient was set to a maximum and the particle contact stiffness to a very low value (theoretically this would lead the biggest angle of repose), the maximum angle that could be simulated was only about 15°. This corresponds to an error of about 53.9 % when compared to the experimental angle of repose, which together with the porosity error is a clear indication that spherical particles by themselves cannot accurately represent a packed bed with irregular shaped particles.

4. Developing a DEM model with irregular shaped particles

The next step was to change the shape and size distribution from purely spherical particles with an equivalent diameter corresponding to 30 mm, to a shape and size distribution which is closer to the actual bed and this was achieved as follow: Ten random rock samples, of five particles each, were collected from the bulk material and visually inspected after which six distinctively different shapes could be identified. Once the groups were identified all the particles were categorized according to the appropriate group, so as to obtain the particle shape distribution or in other words the percentage each shape makes up from the overall sample. During this process the volume of each particle was also recorded so as to establish an overall size distribution.

A three dimensional scan of a single particle out of each group was then obtained and used together with the automatic sphere-clump generator, ASG3D [4], to reconstruct the rock particles using several spheres clumped together (Figure 4). This was necessary, because the DEM software used in this study can only model spherical particles. However, the number of spheres used in ASG3D for the clump reconstruction has to be specified by the user and care should be taken since it directly influences the accuracy of the clumps as well as the computational costs associated with the simulations.

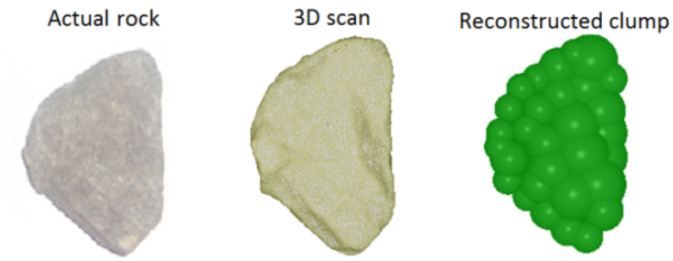

Figure 4: Reconstructing the rock particles with spheres

It was therefore decided to start with 10 spheres per clump and then to repeat the sensitivity study with this newly established particle shape and size distribution. Once again the results were similar to that of the spherical particles (the input parameters had little effect on the porosity), but with two exceptions. The first was that the internal friction coefficient had a much bigger effect on the porosity (Figure 5), than was the case with the spherical particles and the second was that the porosity obtained with the initial input parameters increased to about 0.517. The porosity error therefore decreased from 11.9 % when only spherical particles were simulated to 6.1 % when the reconstructed clumps were simulated.

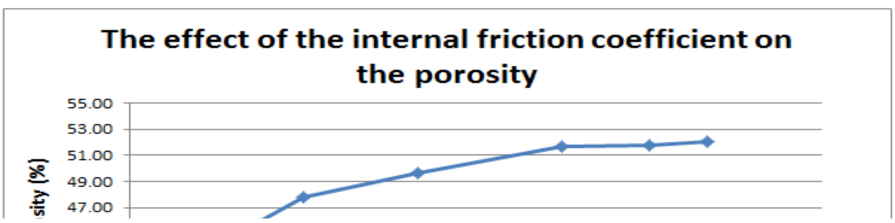

Figure 5: The effect of the internal friction coefficient on the porosity for a bed with non-spherical particles

Two conclusions could be drawn from this result. The first was that as the accuracy of the particle shape and size distribution increased (from purely spherical particles to non-spherical particles), the error associated with the porosity decreased. The second was that even though the porosity error decreased it was still relatively large, which meant that more spheres should have been used during the reconstruction of the clumps. This was verified by simulating the angle of repose experiment again (with the internal friction coefficient set to maximum and the contact stiffness reduced) and the results showed that the maximum angle that could be obtained was about 30°. This was higher that the non-spherical case, but still had an error of 7.7 %.

Nevertheless, the most important aspect to realize is that unlike the previous case, where only spherical particles were used, the experimental porosity and angle of repose can be obtained to within acceptable limits, if the accuracy to which the clumps are reconstructed is improved and if the correct internal friction coefficient is used. The clumps were therefore reconstructed with 35 spheres instead of only 10 and the porosity and angle of repose simulations were repeated. As a result, the porosity shifted to 0.48, while the angle of repose (with the internal friction coefficient set to maximum and the contact stiffness reduced) increased to 35.2°. Since the angle of repose was now higher than the experimental one, it could be assumed that the shapes of the reconstructed clumps were accurate enough and that the internal friction coefficient, which was set to 1.0 (maximum value), simply had to be calibrated. The angle of repose simulations were therefore repeated for several internal friction coefficients (Figure 6), such that the internal friction coefficient which would lead to an angle of 32.5° could be identified. This approach led to an internal friction coefficient of 0.8 and it corresponds to a porosity of 0.485 (error of 0.4%). In order to investigate the effect of increasing the accuracy of the clumps even more, several additional simulations were also performed with 50 and 75 spheres per clump, but the results showed no significant improvements.

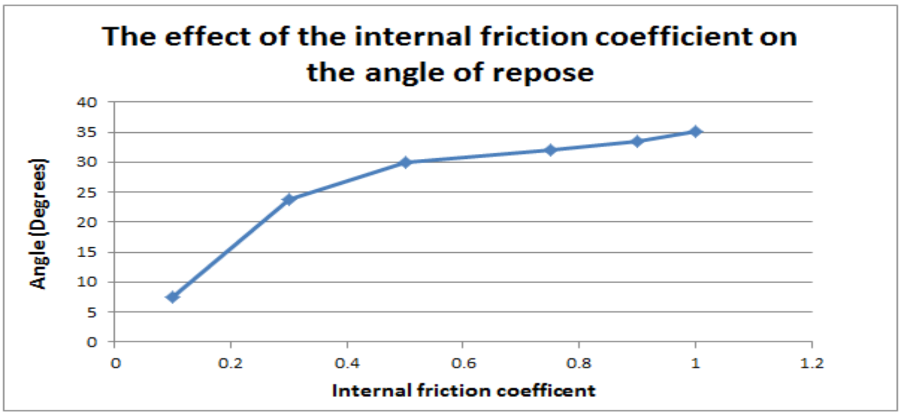

Figure 6: The effect of the internal friction coefficient on the angle of repose for a bed with non-spherical particles

Even though the packed bed used for this study could be modelled accurately, it was relatively small (850 clumps with 35 spheres per clump) and if practical size beds (10,000 clumps with 35 spheres per clumps, for instance) are of interest, further research would first have to be conducted on how to reduce the computational requirements associated with these large models.

5. Converting the developed geometric model

Before any CFD analyses can be conducted the developed geometric DEM models have to be converted into the appropriate format such that they can be imported into the commercially available CFD package, FLUENT [2], for the CFD studies in Part 2 of this paper. In order to achieve this, a Visual Basic Application (VBA) was developed, which is able to reconstruct the DEM models in Autodesk Inventor Professional, such that it can be used to export the model in a STEP file format suitable for FLUENT (Figure 7). One should note that the process displayed in Figure 7 is for a spherical bed, but it is the same for a bed with non-spherical clumped particles.

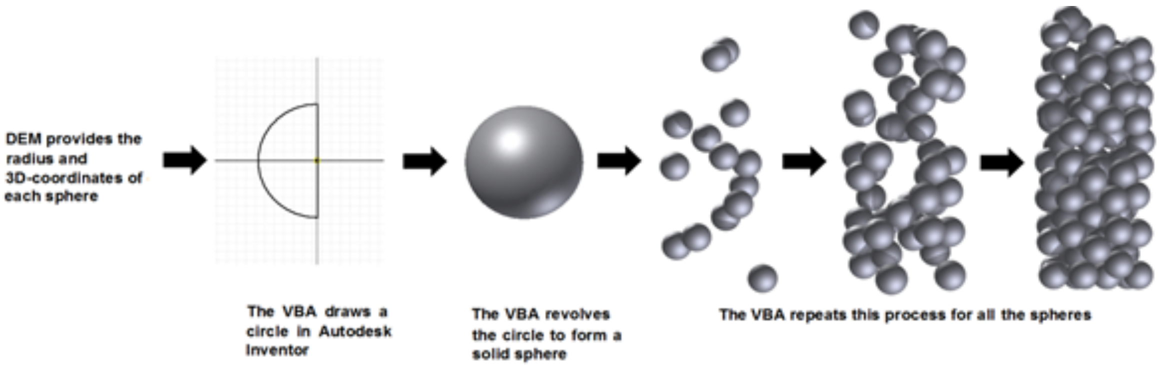

Figure 7: Reconstructing a DEM model in Autodesk Inventor

6. Conclusion

A sensitivity analysis was conducted in order to investigate the degree to which the input parameters would affect the porosity of a DEM model resembling a randomly packed bed with a high aspect ratio and spherical particles. This was to address the issue brought forth by Chung [3], who stated that many authors whom implement a coupled DEM-CFD approach to predict the pressure drop through packed beds, do not adequately justify how they obtained their DEM input parameters. However, the results showed that the input parameters have no significant influence on the bed porosity, except for particles with very low internal friction coefficients. It was also found that a DEM model with spherical particles cannot produce the accurate porosity and angle of repose of an experimental rock bed with irregular shaped particles due to the incorrectly specified particle shape and size distribution. It was therefore necessary to implement some sort of clump logic in order to improve the particle shape and size distribution such that both the experimental porosity and angle of repose could be obtained. This was important, because Part 2 of this paper is focused on developing a method to generate a mesh on a bed with irregular shaped particles such that a CFD analysis can be performed in order to predict the pressure drop over such a bed. Finally, because the DEM software used in this study has to means of exporting the developed geometric model into the appropriate format such that the CFD analysis can be conducted, a possible method to overcome this problem is discussed.

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