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A DEM-CFD APPROACH TO PREDICT THE PRESSURE DROP THROUGH AN AIR-ROCK BED THERMAL ENERGY STORAGE SYSTEM: PART 2 OF 2

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Abstract

The purpose of this paper is to investigate a method to determine the pressure drop trough packed beds using CFD. The focus of this study is on uniform spherical particle. The lessons learned will be extended in the future to irregular shaped particles. The three most important factors examined in this paper are the turbulence model, mesh and geometry. A more detailed investigation into a contact treatment method is presented in this study. The RNG k-□ turbulence model was selected to model turbulence and the interparticle bridge model is selected as a contact treatment method to minimise skew and/or fine cells from forming in the mesh. Further it is recommended that the interparticle bridge diameter should be between 0.2 d_p and 0.3 d_p. The commercial CFD-code ANSYS-FLUENT was used for all simulations.

Keywords: CFD, pressure drop, thermal storage, rock bed

1. Introduction

Solar radiation is considered to be one of the most prospective sources of energy to meet energy demands and prevent the increase of greenhouse gases and climbing fuel prices. To effectively utilise this source of energy, an effective energy storage system must be developed. At present there are several different methods for solar thermal storage, namely sensible storage in liquid, gas or solids, latent heat storage in phase change materials (PCMs) or a combination of these methods. Currently sensible heat storage in liquid materials is used in the solar industry in the form of molten salt [1]. An air-rock bed storage is a possible alternative to molten salt storage. Rock is a non-toxic, non-flammable and inexpensive material. An air-rock storage system allows direct contact between heat transfer fluid and storage material, which eliminates expensive heat exchangers. The large area in contact with the surrounding air flow in a packed bed also results in good thermal performance [2]. The effective heat conduction of the rock bed is low due to the small contact area between the rocks, which aids to lower the heat loss from the packed bed. These characteristic makes an air-rock storage systems an attractive system to investigate further. Ficker [3] did a study based on analytical and experimental work and agrees that rock shows great potential to be a cost effective high temperature storage material, but notes that more research is needed into the thermomechanical behaviour of rocks and pressure drop through a packed bed of rocks.

The Stellenbosch UNiversity Solar POwer Thermodynamic (SUNSPOT) cycle proposed by Kröger, utilises an air-rock bed as a Thermal energy storage (TES) system. This study forms part of a larger project that is investigating the development of porous media approach in computational fluid dynamics (CFD) to simulate flow and heat transfer through an air-rock bed TES system. The porous model will be used as a design tool for the TES for the SUNSPOT cycle. Zavattoni [4] modeled an experimental air-rock bed TES in CFD by representing the packed bed as a porous media. The simulation determined the effect of axial porosity variation on the overall heat transfer. This study showed good comparison with the experimental results and

that including an axial porosity variation distribution into the CFD model, improves the representation of the charging phase and the pressure drop prediction.

To characterise the porous media, three main parameters need to be determined, namely the effective thermal conductivity (particle-fluid heat transfer mechanism), pressure drop (permeability, viscous resistance and fluid velocity) and porosity (arrangement, shape and particle diameter) [4]. To determine these parameters a discrete CFD model of the rock bed will be created and the air flow through the bed will be simulated. According to Lotenburg [5] experimental setups to determine the parameters is limited in their capabilities to determine the heat transfer parameters in a fixed bed according. This limitation is due to the measuring techniques used that disturb the geometry of the bed. Experimental setups are also expensive.

To create a discrete model of the rock bed in CFD, an accurate representation of the geometry of the bed is required. The discrete element method (DEM) is used to generate the packing of the rock particles under the influence of gravity. The rock particles are represented by a clump model which approximates the shape of the rock particle by clumping together a number of spheres. This paper addresses the issue of determining the pressure drop through the packed bed. To help establish a CFD methodology to simulated air flow through a discrete model of a packed bed of irregular particles such as rock, a discrete model of spherical particles is firstly investigated in this study.

2. Previous work

In the past there have been several studies that investigate the use of a CFD or a combined DEM-CFD approach to numerical solve the flow through a packed bed, mostly for the chemical and process industry for fixed bed reactors. Eppinger [6] did a numerical simulation of fixed bed reactors with a small tube to particle diameter ratios. The fixed bed reactor, consisting of randomly packed spherical particles was generated with a DEM-code and the fluid domain was meshed and solved with the commercial CFD-code STAR-CCM+. The predicted porosity and pressure drop was compared to known literature results and agreed well. Ookawara [7] developed a high fidelity DEM-CFD model for process intensification of packed bed reactors. The models porosity and pressure drop compared sufficiently with the Leva and Grummer and Eishfield-Schnitzlein correlation respectively. Delele [8] combined DEM and CFD to investigate the airflow through vented boxes which is used to store horticultural products in cool rooms. The study found that the predicted pressure drop compared well with known correlations. Gunjal [9] did a unit-cell CFD study of a single phase flow in a packed sphere. Fluid flow was simulated through spherical particles in four different structured packing, namely simple cubical, 1-D rhombohedra, 3-D rhombohedra and face-centered cubical. The results show good agreement with the Ergun equation for all four packing structures.

From the previous studies it was determined that the three most important factors to consider when modelling a packed bed in CFD, is the geometry (contact treatment), turbulence modelling and mesh. These three factors are investigated and addressed in this work. The effect of the selected contact treatment method is also investigated in this study.

3. CFD model formulation

Computational power in the last few years has increased enough that it is now possible to numerical solve the flow, mass and energy balance of complex 3-D geometries such as a packed bed using CFD. The geometry of the packed bed is subdivided into a large number of small control volumes, which make up the computational domain (mesh). The larger the number of control volumes in the domain, the more accurate the solution becomes. Boundary conditions must be set for the computational domain. The continuity, Navier-Stokes and energy equations can then be solved iteratively, until the residuals converge [10]. This section discusses the turbulence model, contact treatment and meshing method.

3.1. Turbulence modelling

It is important to know when turbulence occurs, in order to make the decision to use a laminar model or a turbulence model in a CFD simulation. According to Eisfeld and Schintzlein [11] the flow regime in packed beds is defined by the particle Reynolds number $Re_p = \rho U_0 d_p/\mu$. Where ρ is the fluid density, U_0 is the superficial velocity, d_p is the particle diameter and μ is the fluids viscosity. The laminar, transitional and fully turbulent flow regime occurs at $Re_p < 10$, $10 \leq Re_p \leq 300$ and $Re_p > 300$ respectively [11].

A time depended solution of the Navier-Stokes equation for a high Reynolds number turbulent flow in complex geometries such as packed beds is currently above our computational capabilities. To avoid directly simulating the small scale eddies, two methods have been developed that transform the Navier-Stokes equation. The one method is Reynolds Averaging (RANS) and the other is Large-Eddy simulations (LES). Both of these methods add additional terms that need to be solved [12]. LES requires more computational power and has not been used extensively in CFD simulation of packed beds. Coussirat [13] mentions that it is currently not computationally affordable to use LES. RANS turbulence models such as the k-□ (standard, renormalized group and realizable), k-ω and Spalart-Allmaras (S-A) have been extensively used in previous packed bed CFD studies. The following equations are the RANS governing equation in Cartesian coordinates used in this study, for steady-state incompressible flow in the absence of external forces. The energy equation is disabled for all simulations in this study.

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

$$\rho\left(u_j \frac{\partial u_i}{\partial x_j}\right) = \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho \frac{\partial(-\overline{u_i' u_j'})}{\partial x_j} \tag{2}$$

Where u_i and u_j represent the fluid mean velocity components in the x, y and z directions. The subscripts i and j represent the Cartesian coordinate index. The Reynolds averaged values and the effects of the turbulence are represented by the Reynolds stresses which is the last term in equation (2) and are approximated by the Boussinesq hypothesis:

$$-\overline{u_i' u_j'} = \frac{\mu_t}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3} k \delta_{ij} \tag{3}$$

Where μ_t is the turbulent viscosity. To compute turbulent flows using the RANS equation it is necessary to use turbulence models to predict the Reynolds stresses [14]. Several studies have modelled turbulence in packed beds. Gunjal [9] used the Reynolds-averaged Navier-Stokes equation along with the standard k-□ turbulence model to account for the turbulent stresses. Transition flow regime was modelled as turbulent flow because of the uncertainties in simulating transitional flow regimes in a complex geometry. Guardo [15] did a study to determine the most accurate RANS turbulence model for wall-to-fluid heat transfer in a packed bed. It showed that the k-□, k-ω and S-A turbulence models all predicted the pressure drop accurately according to the Ergun equation. Lee [16] investigated turbulence induced heat transfer in the packed bed of spheres of a PBMR core using LES and RANS. The k-ω model from the RANS turbulence models and the LES was selected to model the turbulence. It was found that the LES predicted a higher pressure drop, a more random flow field, a higher vortices magnitude and higher temperatures at local hot spots on the pebble surface than the k-ω RANS turbulence model. Nijemeisland and Dixon [10] used the renormalized group (RNG) k-□ turbulence model selected to model the turbulence and the RNG k-□ model is more responsive to strain and streamline curvature. Eppinger [6] used the realisable k-□ turbulence model and 'all y^+ treatment' to model the turbulence in his study.

The RNG *k*-□ turbulence model is selected to model the turbulence in the packed bed. The RNG *k*-□ model is derived from the instantaneous Navier-Stokes equation using a mathematical technique called the renormalized group method. The model is similar to the standard *k*-□ model, but has different constants and

additional terms and functions in the turbulent kinetic energy (k) and turbulent dissipation (ε) transport equations. The turbulent viscosity is defined identically to the Standard k-ε model [17].

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{4}$$

The difference is the constant C_μ, which is 0.0845 for the RNG k-ε model, and 0.09 for the standard k-ε model. The transport equations for the RNG k-ε model has a similar form to the standard k-ε model.

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j}\right) + \mu_t S^2 - \rho\varepsilon \tag{5}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left(\alpha_\varepsilon \mu_{eff} \frac{\partial \varepsilon}{\partial x_j}\right) + C_{1\varepsilon}\frac{\varepsilon}{k}\mu_t S^2 - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} - R_\varepsilon \tag{6}$$

The quantities α_k and α_ε are the inverse Prandtl number for k and ε respectively. The constants $C_{1\varepsilon}$ and $C_{2\varepsilon}$ are derived analytically by the RNG theory and are 1.42 and 1.68 respectively. The last term in equation 6 is the major difference between the Standard and RNG k-ε models. This terms gives a lower turbulent viscosity in rapidly strained flows which makes the RNG model more responsive to the effect of rapid strains and streamline curvature [17]. Nijemeisland and Dixon suggested that this feature of the RNG model makes it more suitable for complex flows where the streamline must curve around particles.

3.2. Wall function

The presence of a solid surface strongly effects turbulent flows and special conditions need to be set. Several methods do exist to resolve the flow near a solid surface. The boundary layer can be directly resolved by using a highly refined mesh near the solid wall or the near wall region flow can be solved by an empirical model. Directly modelling the boundary layer can result in expensive computational resource in a packed bed, because of the large surface area of the wall and particles. Using a wall function can eliminate the need for expensive computational resources [12]. A wall function is a set of semi-empirical formulas and functions and comprises of the law-of-the-wall and formulae for the near wall turbulent quantities [17]. Gunjal [9] used various wall functions for the turbulent simulation, the standard wall function, enhanced wall function, and non-equilibrium wall function. There was however no significant influence by the choice of wall functions according to his study. Nijemeisland and Dixon [10] used the non-equilibrium wall function to model the vicious sublayer and transition region. This wall function is also selected to model the near wall region in this study. It is recommended for use in complex geometries where separation, reattachment and impingements where the mean flow and turbulence are subjected to pressure gradients and rapid changes occur. Improvements can be obtained in prediction of the wall shear over using the standard wall function [17].

3.3. Contact treatment

Contact treatment is a crucial factor when trying to model a packed bed in CFD. Mathematically a contact point has an area of zero. Therefore to represent it mathematically with a mesh would require infinitely fine or highly skew cells. Very fine cells could lead to a large computational cost and very skew cells could cause convergence problems [6]. Several methods to overcome this problem exist in literature. Augier [18] did a numerical simulation of transfer and transport properties inside packed beds containing spheres. The method used in this study to eliminate contact points was to contract the diameter of each particle in the bed by 2 %. This allowed the cells to be generated between the particles, but the contraction reduced the solid fraction of the bed, and therefore a porosity correction and pressure drop correction was required. Another method is to enlarge the particle diameter so that the particles overlap each other in the vicinity of the contact point, thus eliminating the contact point by replacing it with a contact line. This allows cells to be generated around the contact lines. However this also changes the solid fraction of the bed and a porosity and pressure drop correction is also required [7]. Eppinger [6] resolved the contact point problem by flattening the particle in the region of the contact point and also particles in near contact with each other or the wall. This allowed cells to be generated between the particles. This method caused only a small modification to the geometry

and as a result did not require any correction for the porosity and pressure drop. Ookwara [7] connected the particles in contact with each other or the wall or in near contact with a circular cylindrical bridge. This method was referred to as the interparticle bridge model. This resolved the problem of fine cells and skew cells being generated around the contact point. The study assumed that the cylindrical bridge existed in the stagnation region observed experimentally and numerically by Suekane [19] and Gunjal [9] respectively in the region of the contact point. The study concluded that macroscopic flow properties such as the pressure drop is not affected by the cylindrical bridge between the particles. No information was provided about the effect of the interparticle bridge on the porosity [7]. The interparticle bridge model is selected to treat the contact points in the packed bed. This method is further investigated in this study to determine the influence of the diameter size of the circular cylindrical bridge (d_b) between the particles on the porosity.

3.3.1 Interparticle bridge model

The pressure drop of a packed bed is significantly influenced by the global porosity and it is an important factor for the accuracy of the prediction [6]. Three structured packing's and one random packing was used to determine the effect of the interparticle bridge model on the porosity. The structured packing's used are simple cubic ($\varepsilon = 0.48$), body centred cubic ($\varepsilon = 0.32$) and face centred cubic ($\varepsilon = 0.26$). The discrete element method is used to generate a randomly packed bed consisting of 400 spherical particles contained in a circular cylinder ($\varepsilon = 0.42$). The cylinder has a diameter 0.24 m and the particle has a diameter of 0.03m. The predicted coordinates of the particles are then used to generate a CAD model in Autodesk inverter 2011, where each particle is created and also automatically bridged. The particles are bridged when they are in contact with each other or the wall or in near contact with other particles. The structured packing's only use particle-to-particle bridging. The solid volume V_s of the packed bed is calculated in Autodesk Inverter 2011 and the void volume V_v is calculated by subtracting V_s from the cylinder volume V_c , which has a height equal to the packing height of the particles. The porosity is then calculated by $\varepsilon = V_v/V_c$. Figure 1 below shows how the particles are bridged with the other particles and the wall.

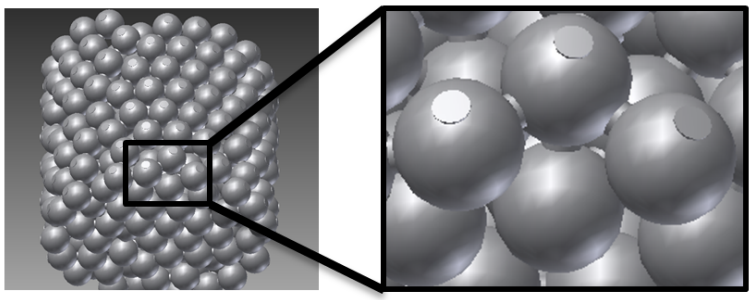

Figure 1: Interparticle bridge model (Autodesk Invernter 2011)

Figure 2 shows how the porosity error increases as the bridge to particle diameter ratio (d_b/d_p) increases.

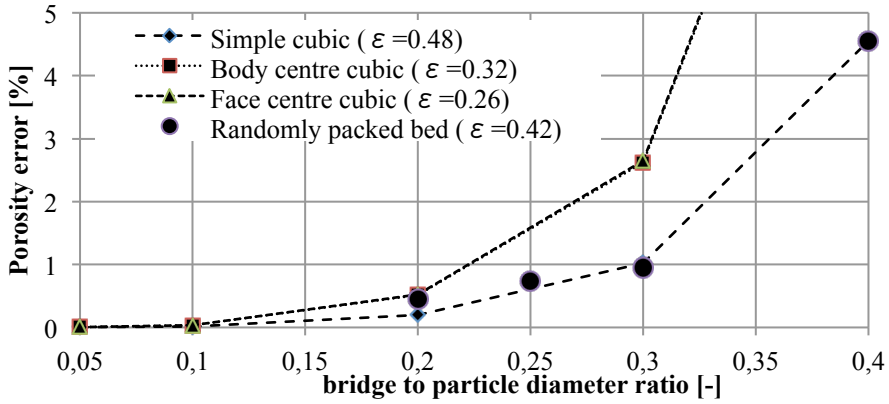

Figure 2: Effect of the interparticle bridge model on the global porosity

The interparticle bridge model causes the porosity to decrease. This is expected because the bridge model adds material which increases the solid fraction. From the graph it is seen that the porosity error increases considerably above $d_b/d_p = 0.3$ for all packed structures. The effect of the bridge model in the porosity is greater for denser packed structures. This analysis is done only for beds with uniformed size particles, a bed containing non-uniform particles could lead to different results.

3.4 Mesh

The construction of the mesh is an important part in CFD modelling, especially in complex geometries. The accuracy is strongly affected by the mesh and it must be selected with enough detail to describe the flow accurately, but coarse enough to complete the simulation in reasonable time. There exists two main types of mesh namely structured and unstructured. Unstructured mesh is more suitable for complex geometries such as those found in packed beds. The thickness of the cell near the wall expressed in terms of y^+ is preferred to be greater than 30 for the proper use of the wall function. This is however difficult in packed beds where small gaps are present that constrains the cells size. This introduces systematic errors in the predicted pressure drop that is initially hard to access [20].

Several mesh specifications for packed beds was found in the literature. Dixon et al. used an average cell size of 0.5-1 mm for particle of a 25.4 mm in diameter. Freund et al. [21] used a grid size of $d_p/30$. Eppinger et al. [6] specified a surface mesh size and then generated the volume mesh based on the surface mesh. The triangle edge size for the surface mesh of the particles were 4-10% of the particle diameter. Two boundary layers were used with a thickness of 3% of the particle diameter. Delele et al. [8] used a grid size of 5 mm for the surface mesh of the particles ranging in diameter between 65 and 75 mm. After comparing calculated results and computational time of different meshes, a particle surface mesh size of between 1.8 mm and 2 mm was selected. The volume mesh is generated based on the surface mesh of the particles. The selected sizes 6-7 % of the particle diameter, falls in the range that Eppinger used. A tetrahedral mesh is used.

4. CFD simulation

The CFD simulation was done for the randomly packed bed with a 0.2 d_p and 0.3 d_p diameter interparticle bridge model. The geometry and fluid domain is shown below in Figure 3.

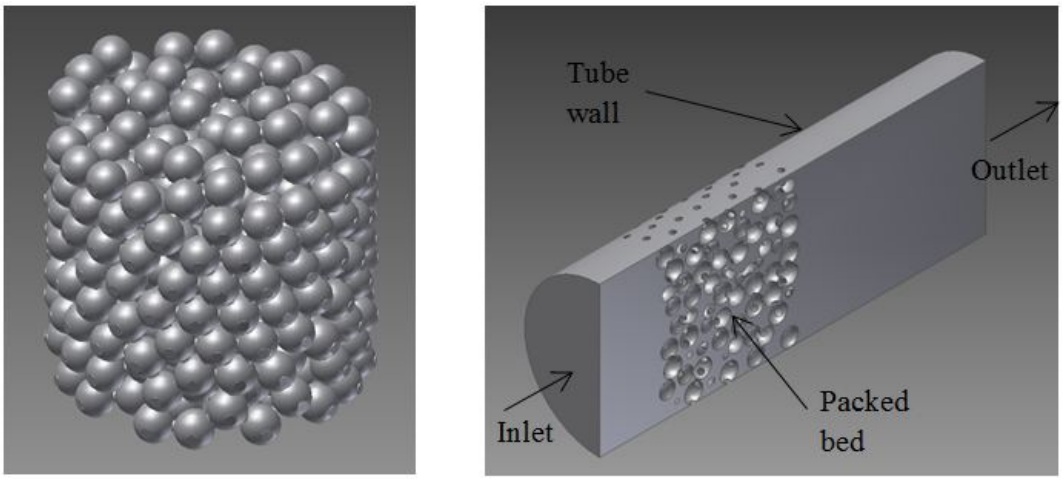

Figure 3: Packed bed geometry (Autodesk inverter 2011)

The boundary at the inlet and outlet is extended by 3 and 10 particle diameters respectively, to minimize the effect of the boundary conditions [6]. It is found that if the diameter of the bridge model is below 0.2 d_p, fine or skew cells are generated around the bridge model, increasing the mesh size considerably.

The commercial CFD-code ANSYS-FLUENT is used for the simulation which is based on the finite volume method. The fluid flowing through the domain was assumed to be incompressible with physical properties of air at 300 K ($\rho = 1.1767 kg/m^3$; $\mu = 1.8557\times10^{-5}$). The flow through the model was done in the laminar (Re_p=1), transitional (Re_p=100) and turbulent (Re_p=1000) regime. The turbulence was modelled with the RNG k- □ model and the near wall region with the non-equilibrium wall function. The pressure-velocity coupling was done using the SIMPLEC algorithm. All the spatial discretisation was done using the second order upwind scheme. The boundary condition for the inlet, outlet and wall and particle surfaces was set as a velocity-inlet, pressure-outlet and non-slip solid wall boundaries respectively. The simulation was done until the pressure at the inlet converged. The number of cells of the mesh was around 5.6 million. The simulation's time was between 7h-10h. All the CFD simulations were done using an Intel i7 870, 2.93GHz processor with 16 GB of RAM.

4.1 Pressure drop

The predicted pressure drop was validated using the Eisfeld and Schnitzlein equation [11]. The friction factor f is defined as shown below in equation 7.

$$f_{ES} = \left(\frac{\Delta P}{\rho U_0}\right)\left(\frac{d_p}{L}\right)\left(\frac{\varepsilon^3}{1-\varepsilon}\right) = 154 \cdot {A_w}^2 \frac{(1-\varepsilon)}{Re_p} + \frac{A_w}{B_w} \tag{7}$$

$$A_w = 1 + \frac{2}{3(D/d_p)(1-\varepsilon)} \quad B_w = \left[1.15\left(\frac{D}{d_p}\right)^2 + 0.87\right]^2 \tag{8}$$

The Eisfeld and Schnitzlein equation takes into acount the particle-to-tube diameter.The results compared sufficiently with the Eisfeld and Schnitzlein equation as shown in Figure 4. There is no significant difference noticed in the pressure drop between the 0.2 d_p amd 0.3 d_p diameter bridge model. The deviation of the 0.2 d_p bridge model for the lamanar, transitional and turbulent flow regime is 2.4 %, 8.5 % and 25 % repsectivly. The maximum deviation between results of the 0.3 d_p bridge models and the 0.2 $d_p$bridge model

is 6.1 % and found in the turbulent regime.

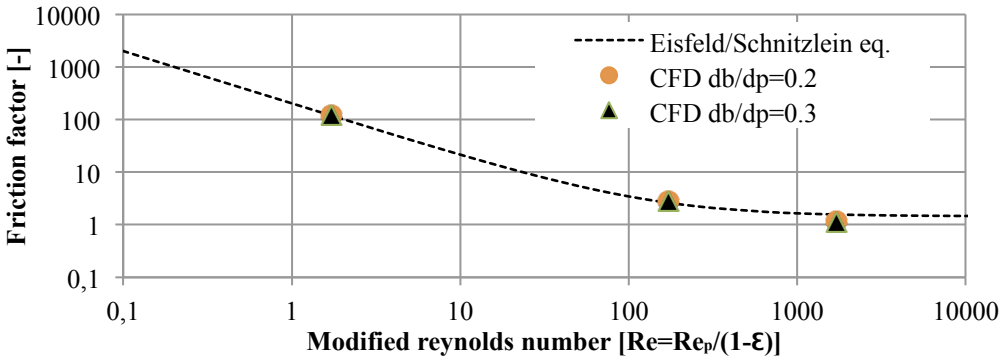

Figure 4: Effect of the interparticle bridge model on the global porosity

It seems reasonable to argue that at d_b/d_p=0.3, the bridge models exits in the stagnation region and does not affect the macroscopic flow properties.

5. Conclusion

From previous CFD studies done on packed beds, it was determined that the three most important factors are the geometry, turbulence model and mesh. The interparticle bridge model was selected to treat the contact points in the bed, which minimised the generation of very skew and fine cells in the contact region. The RNG k-□ turbulence model was selected to model the turbulent flow through the packed bed, because it is more responsive to stream line curvature and the effect of rapid strain. The size of the inter particle bridge model increased the solid fraction of a packed bed. The porosity investigation showed that the error increases significantly above 0.3 d_p. It is recommended that the bridge model diameter should be smaller than 0.3 d_p. To minimise the generation of fine cells it is recommended that the bridge model diameter should be above 0.2 d_p.

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