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ANALYTICAL SCALING OF DEM PARTICLES FOR EFFICIENT PACKED-BED SIMULATIONS

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ABSTRACT

Packed and Fluidized beds are commonly found in industries such as chemical processing and refining. A major advantage to these configurations lies in the large solid-surface area exposed to the flow, allowing for rapid interaction between the solid and fluid phases. While these types of flow configurations have been heavily studied over the years, computational software and hardware are only recently becoming advanced enough to allow realistic simulations of industry relevant configurations. Recent developments have allowed for the coupling of Discrete Element Modeling approaches, where conservation equations are typically solved on a particle-by-particle basis, with traditional continuum-fluid dynamics simulations. Nonetheless, when fluid-particle interaction is important, such as in packed bed analysis, modeling of the individual particles may still be computationally prohibitive except for simple applications. Methods to improve computational costs include grain coarsening or parcel-based approaches, where particle sizes may be scaled up or groups of particles are treated statistically. The present study develops and validates an analytical approach for the scaling of the Coefficient of Drag equations in a simplified packed bed simulation with scaled-up particles, using CD-adapco's STAR-CCM+ software. Pressure drop predictions are compared against the accepted Ergun Correlation for the high density cylindrical packed bed. Container contact forces and packed bed height are also monitored as the flow rate is increased toward fluidization. It is shown that by properly scaling the Coefficient of Drag, while doubling the particle diameter (effectively reducing the total number of simulated particles by 8), a more than 15X speed-up in simulation time is achieved. This speed-up is achieved with an increase in error of only 8% maximum for the cases studied. Additionally, similar physical behavior is observed between the cases. This analytical approach proves to be a robust method of reducing computational expense without sacrificing accuracy, effectively making industrial scale simulations feasible.

INTRODUCTION

With the use of packed and fluidized beds becoming more common in industrial applications, there has been an increasing need for advanced design tools. Fixed beds packed with spherical particles, in particular, are used in a variety of industries; with applications including grain dryers, catalytic reactors, absorbers, and filters [1]. Design characteristics of interest typically include the pressure drop behaviour among others.

NOMENCLATURE

A	[m^2]	Projected Area
C_d	[-]	Particle drag coefficient
d	[m]	Particle diameter
F_{drag}	[N]	Drag force on a DEM particle
F_p	[N]	Force exerted on DEM particle due to pressure gradients
f_p	[-]	Friction factor in a packed column
L	[m]	Packed bed length
$\dot{m}$	[kg/m^3]	Mass flow rate
N	[-]	Number of particles
Re	[-]	Reynolds Number
t	[s]	Simulation run time
u	[m/s]	Fluid Velocity
v	[m/s]	Particle Velocity
V	[m^3]	Volume
V_s	[m/s]	Superficial Velocity
Special characters		
α	[-]	Void fraction ratio
Δp	[Pa]	Pressure gradient
μ	[Pa*s]	Dynamic viscosity
ρ	[kg/m^3]	Density of fluid
Subscripts		
p		DEM particle based value
f		Fluid based value
i		Inlet based value
1x		Values for the full scale DEM simulation
scaled		Values for the scaled DEM simulation
r		Ratio

A great deal of literature exists in regard to the prediction of the pressure drops in Packed and Fluidized beds [2-8, for example], ranging from empirical to analytical correlations. Many traditional fixed beds are cylindrical columns filled with spherical particles, applications where the existing predictive methods provide adequate accuracies. For example, the Ergun equation, defined in a later section, is routinely utilized to predict pressure drops in high density fixed bed flows [9]. In fact, much of the existing work treats the fixed bed as a porous media, again with adequate levels of accuracy. However, as designs become more advanced and complex, new design tools are required [10]. These tools must not only accurately predict the performance of the more advanced configurations being developed, but also provide further insight into the performance. For example, dynamic information such as transient forces and trajectories can be readily obtained with recently available tools. For these reasons, computational techniques involving Discrete Element Modeling (DEM) are becoming increasingly popular.

Improvements in numerical methods and computational hardware have made simulations of the Particle Bed-Fluid interactions feasible through the coupling of DEM simulations with Computational Fluid Dynamics (CFD) simulations [11]; to the point where user friendly tools are commercially available as part of CAE software. For example, the CAE tool STAR-CCM+, allows for the implicit two-way coupling described above [12]. With these capabilities, users are able to simulate real-world geometries and scenarios, while exposing an invaluable amount of additional physical details. Limitations still exist, nonetheless, as the computational expense of these types of simulations is proportional to the particle count and inverse of the particle diameter [13]; often leading to prohibitively excessive solution times for realistic models. This effect is compounded when fluid-particle coupling is included.

Engineers have come up with various methods to overcome this hurdle in practice; involving reduction of the computational domain, or more commonly scaling of particles. In order to maintain the expected behaviour of a full scale particle, scaled particles are often modelled with modified properties. A variety of approaches have been proposed to achieve the similarity between full scale and scaled models, such multi-scale models, parcel-based approaches, and grain coarsening [11, 13-15, for example].

The present study intends to investigate the ability to analytically modify the utilized Drag Coefficient correlation, a parameter available to the user in CD-adapco's STAR-CCM+ CAE tool (v8.04.010), based solely on the scaling factor's geometric implications. The accuracy of this approach will be assessed by comparing results against the established Ergun equation for a range of flow rates through a fixed, densely-packed bed. It is expected that this approach will serve as an accurate and straightforward method for achieving improvements in computational costs, resulting in a greater use of higher fidelity simulations in the design process.

COMPUTATIONAL DOMAIN & SET-UP

In order to assess the accuracy of the proposed scaling approach, a simple cylindrical packed bed was analysed, as shown in Figure 1. The cylindrical domain modelled was 25 mm in diameter and 169 mm tall, oriented with the cylinder axis parallel to the gravitational vector. Particles of 1.6mm diameter were utilized for the full-scale simulations. Mechanical properties of the particles matched those of Aluminium; yet do not have a significant impact on the results of this fixed bed simulation.

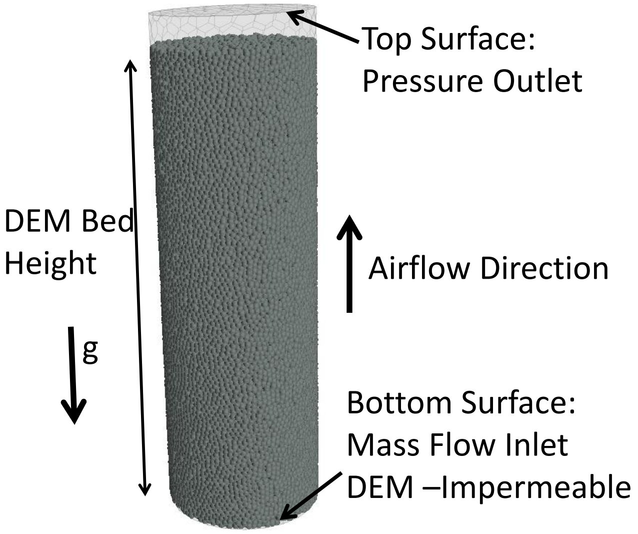

Figure 1: Computational Domain filled with Full Scale Particles

The walls of the cylinder were also modelled using Aluminium material properties, when considering their interaction with the DEM particles. Of importance was the defined coefficient of rolling resistance, left as default values for the materials chosen: 0.1. The top surface was configured as a Static Pressure Outlet, set to atmospheric pressure. The inlet was defined as a mass flow inlet, impermeable to the DEM particles.

A range of inlet mass flows, and therefore superficial velocities, was tested with the intention of increasing velocities until the bed begins to fluidize.

Prior to simulating the packed bed, the particles are introduced by allowing them to enter through the top of the domain, with the bottom surface set as impermeable to the DEM particles. Particles were injected until the domain was filled to approximately 152 mm in height, at which point the injector was disabled. The simulation continued to run, with a reduced DEM time step, such that all of the kinetic energy could be drained from the particles, and the maximum particle velocity sufficiently approached zero.

Reported results will include pressure profiles along the bed, inlet pressures, average superficial velocity, and the sum of the forces on the bottom surface of the domain, as well as bed height. The pressure profile along the domain is taken as the spanwise averaged pressure along the symmetry plane, as shown in Figure 2.

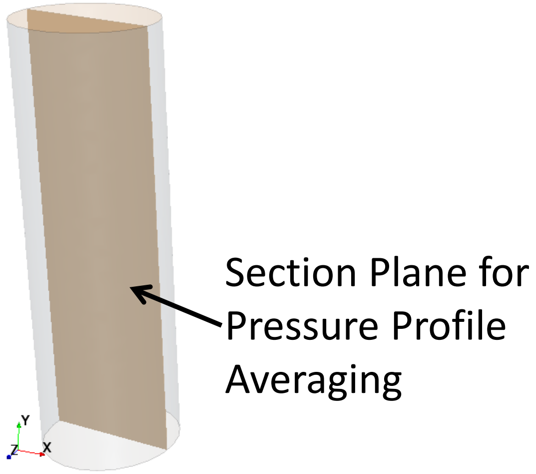

Figure 2: Section Plane for Pressure Profile Averaging

NUMERICAL METHOD

The CAE tool utilized in this study, STAR-CCM+, utilizes a fully 3-dimensional, Navier-Stokes finite volume methodology for simulation of the fluid flow; with a great deal of literature available regarding the details [12]. Particle behaviour is simulated with a soft-sphere approach, involving the direct integration of each spherical three-dimensional equations of motion. Again, a great deal of literature is available describing the details of this approach [13].

In order to satisfy numerical requirements for DEM-CFD coupling, the generated mesh was created with cells larger than the particle size, such that local solid and void fractions can be calculated during each iteration of the fluid solver.

The fluid domain was solved using an unsteady Laminar flow model with DEM 2-way coupling enabled. This effectively captures the impact the flow has on the particles and vice-a-versa, essential for these types of calculations. The unsteady simulation included enough time steps such that the flow had enough time to pass through the domain at least twice, according to the following equation:

$$t \geq 2 * \left(\frac{L}{V_s}\right) \tag{1}$$

Additionally, the particle velocities, bed height, and inlet pressure were all monitored to ensure values were no longer changing with respect to time.

Of particular importance for the current work is the manner in which the drag forces are calculated in a packed bed simulation. Fluid-Particle coupling is achieved through the momentum transfer between phases. The fluid provides the momentum to particles through the application of drag force and pressure gradient force. At the same time, the sum of all vectors of fluid forces on particles for all particles inside each volume cell, are contributing to the momentum source term in the Navier-Stokes equation.

The force F_{fluid} has contributions from drag force F_{drag} and pressure gradient force F_p

$$F_{drag} = \frac{1}{2}\rho C_d A_p |u - v|(u - v) \tag{2}$$

$$F_p = \Delta p V_p \tag{3}$$

Here ρ_f is fluid density, C_d is drag coefficient, A_p is projected area of particle, u is velocity of fluid, v is velocity of particle, ∇p is pressure gradient, V_p is volume of particle. As the present study was concerned only with densely packed fixed beds, the Gidaspow approach is utilized for C_d calculations [16], which reduces to the Ergun equation at high solid densities. In particular,

$$C_d = \frac{4}{3}\left(\frac{150(1-\alpha_p)}{\alpha_p Re_p} + 1.75\right) \tag{4}$$

Here α_p is void fraction, Re_p is particle Reynolds number, α_p is the local void fraction. Drag coefficient depends on particle size through the definition of particle Reynolds number

$$Re_p = \frac{\rho|u-v|d}{\mu} \tag{5}$$

Where μ is the dynamic viscosity of the fluid.

With the version of STAR-CCM+ utilized in the present study (v8.04), the user is able to modify the calculated drag force solely through modification of the utilized drag coefficient. Additionally, the drag coefficient defined above is available to the user as a built in field function. Therefore, the user can potentially modify the previously defined drag coefficient by an appropriate scaling factor. In fact, this approach has been taken in the past [13], using a pseudo-empirically based modification factor. In the present study, the authors intend to utilize an analytically defined scaling factor, based solely on the particle scaling ratio.

As noted, the particle size is accounted for in the definition of the particle Reynolds number, which was not user-definable in this version of STAR-CCM+ (later versions include this capability). Additionally, the particle's size is accounted for in the area of the particles, when computing the resulting force and momentum source.

To compare the resulting pressures against accepted predictions, results will be compared to predictions made with the Ergun equation applied to the packed bed as a whole, defined as [3]:

$$f_p = \frac{150}{\frac{d * V_s \rho}{(1-\alpha_p) * \mu}} + 1.75 \tag{6}$$

$$f_p = \frac{\Delta p}{L} * \frac{d}{\rho {V_s}^2}\left(\frac{{\alpha_p}^3}{1-\alpha_p}\right) \tag{7}$$

From the above equations, all variables are extracted as averaged values from the simulated domain, ensuring an accurate comparison between simulation and predictions. In the case of void fraction calculations, for example, the average void fraction was calculated using the built in functionality within STAR-CCM+, from a volume including that only of the bed volume (i.e. excluding the 17mm of unfilled space above the particle bed).

With the flow and bed characteristics calculated, the only remaining unknown, Δp, is solved for. Hence, for each test condition, a predicted pressure drop across the packed bed is available.

The superficial velocity (V_s), used in the Ergun equation, is the equivalent velocity through an empty cylinder of equal volumetric flow rate. It is defined as:

$$V_s = \frac{\dot{m}_i}{\rho * A_i} * \alpha_p \qquad (8)$$

Analytical Scaling Method

As mentioned, the focus of this paper is to explore an analytical approach to the scaling of the utilized coefficient of drag correlation. With control only over this correlation, and access to local variables and predefined drag correlation estimates, it is necessary to develop a scaling parameter that accounts for the increased particle size, and reduced overall number of particles. With acceptable accuracy, this approach will provide a powerful tool allowing for improved computational efficiency in industry relevant DEM-packed bed simulations.

In this analysis, we are interested in defining a drag coefficient such that the effective pressure drop in a scaled simulation is equivalent to that of a full scale simulation.

We define the simulated drag coefficient, calculated using the Gidaspow correlation and the simulated (scaled) particle dimensions and local flow quantities, as $C_{d,scaled}$. Similarly, we define the full scale drag coefficient, calculated using the Gidaspow correlation and the full scale particle size and flow quantities as $C_{d,1X}$, we can then state, assuming the void fraction is equal between the two cases:

$$C_{d,scaled} = \frac{4}{3}\left(150 * \frac{1-\alpha_p}{\alpha_p * Re_{p,scaled}} + 1.75\right) \qquad (9)$$

$$C_{d,1X} = \frac{4}{3}\left(150 * \frac{1-\alpha_p}{\alpha_p * Re_{p,1X}} + 1.75\right) \qquad (10)$$

The ratio between these drag coefficients can be related to the calculated particle Reynolds number as:

$$\frac{C_{d,scaled}-1.75}{C_{d,1X}-1.75} = \frac{Re_{p,1X}}{Re_{p,scaled}} = \frac{d_{1X}}{d_{scaled}} = d_r \qquad (11)$$

Therefore the drag coefficient which would replicate that of the full scale bed can be defined in terms of the scaled drag coefficient as:

$$C_{d,1X} = {d_r}^{-1} * C_{d,scaled} - 1.75 \qquad (12)$$

The equation above accounts for the difference in particle size as it applied to the particle Reynolds number; in effect the drag coefficient used in determining the drag force and ultimately the momentum source acting on the fluid. However, the overall drag force, defined in Equation 2, is also affected by the particle size in the A_p calculations. Therefore, an additional term is required to relate the individual and total particle areas in the full scale model to the scaled model. As the user must account for these effects through the utilized drag coefficient correlation, the additional terms will be multiplied by the above drag coefficient equation, $C_{d,1X}$, as follows:

$$A_r = \frac{A_{1X}}{A_{scaled}} * \frac{N_{p,1X}}{N_{p,scaled}} = {d_r}^{2} * {d_r}^{-3} = {d_r}^{-1} \qquad (13)$$

Hence, the drag coefficient utilized in the scaled simulation, would be defined as:

$$C_{d,input} = C_{d,1X} * {d_r}^{-1} = {d_r}^{-1}\left({d_r}^{-1} * C_{d,scaled} - 1.75\right) \qquad (14)$$

This is the definition of the drag coefficient input into the STAR-CCM+ model, with $C_{d,scaled}$ being available as a built in field function calculated using the Gidaspow correlation on the simulated particles.

Test Matrix

The test matrix for the current study was developed in order to ensure the proposed scaling method is applicable through the full range of superficial velocities, up until the bed becomes fluidized. This will be observed by a distinct increase in bed height and reduction in the total force on the bottom surface of the domain. This sweep of inlet conditions was repeated for the scaled approach. The current study utilized a scaling factor of 2X, with the particles being twice the diameter of the full scale particles. The domain size was maintained, and the mesh was adjusted such that proper void fractions were maintained in each cell. The test matrix can be seen below in Table 1, along with the respective case designations.

Table 1: Test Matrix for the current study, along with extracted bed properties and Ergun Predictions

Case (1X Scale)	$\dot{m}_i$(g/s)	$\alpha_{p,i}$	V_s(m/s)	α_p	**ΔP_Ergun** (Pa)
1	0.613	0.439	0.271	0.388	413.75
2	0.723	0.444	0.320	0.389	521.12
3	0.833	0.448	0.368	0.392	636.78
4	0.957	0.457	0.423	0.390	772.91
5	1.077	0.463	0.476	0.390	918.38
6	1.208	0.472	0.534	0.398	1133.04
Case (2X Scale)					
1_2x	0.673	0.482	0.298	0.408	387.30
2_2x	0.784	0.481	0.347	0.408	480.42
3_2x	0.908	0.488	0.402	0.408	594.55
4_2x	1.035	0.495	0.459	0.408	723.17
5_2x	1.155	0.498	0.512	0.407	854.72
6_2x	1.238	0.483	0.548	0.414	901.40

In Table 1 above, boundary conditions, superficial velocities, void fraction, and Ergun predictions for the bed are given. The area averaged inlet surface void fraction is also provided, as this value affects the inlet boundary condition slightly by not allowing flow through locations where the solid phase resides. Hence there are slight differences between the full scale and 2X scale cases. However, as Ergun predictions are made in-situ, from values extracted from the simulation, as opposed to nominal values, the approach and comparison is still valid. Figure 3 compares the filled domain for the full scale model with that of the scaled model.

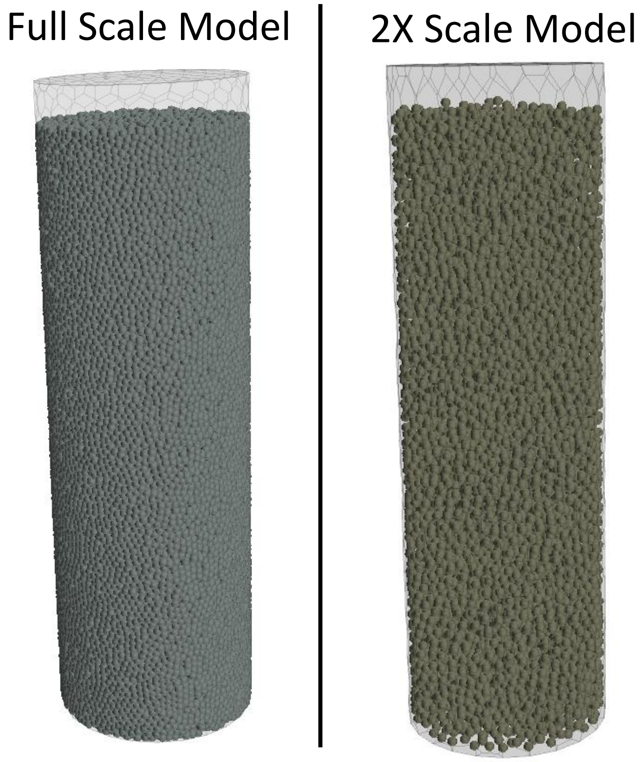

Figure 3: Comparison of Full Scale and 2X Scale Models

FULL SCALE RESULTS

Before assessing the accuracy of the scaling approach described above, it is necessary to first benchmark STAR-CCM+'s ability to match the Ergun predictions at full scale (ie. no modification of the built-in Gidaspow drag coefficient correlation). Considering case 1 first, the resulting pressure profile along the cylinder can be seen in Figure 4.

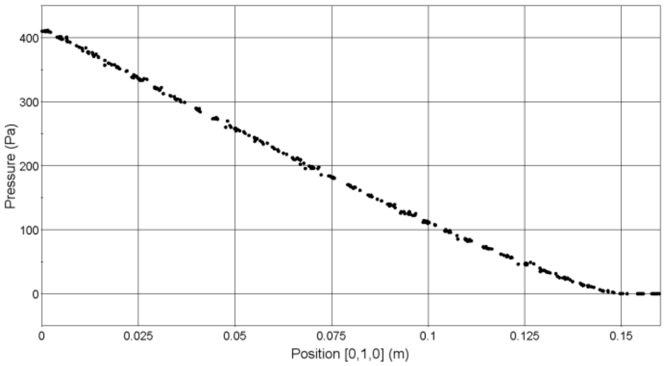

Figure 4: Full Scale Pressure Profile - Case 1

From Figure 4, we see the pressure behaves as expected for the full scale case. A large pressure drop is seen across the bed, with a negligible pressure drop across the empty section of the domain. Additionally, from the Ergun equation above, we see that the expected pressure drop is expected to be a linear with respect to the bed length, as is seen here. The remaining cases exhibited similar behaviours.

The contact forces on the bottom surface of the domain were also examined, in order to identify the point at which the packed bed was beginning to fluidize. This is identified as the point at which the contact force sufficiently approaches zero. These results are shown in Figure 5. One immediately notices the forces are negative for all cases, as they are expected to be directed in the direction of gravity. Additionally, the force magnitudes monotonically decrease as the superficial velocity is increased. This again is expected, as the forces exerted on the particles counter those forces imposed by the gravitational acceleration. Finally, as the flow rate is increased to Case 6 ($V_s = 0.534$), the contact force is essentially zero (-0.016N), suggesting the bed has become fluidized. Additionally, a bed height increase of 2.2mm was observed for this case, again confirming the bed has sufficiently fluidized beyond the point where one would be comfortable applying the Ergun prediction.

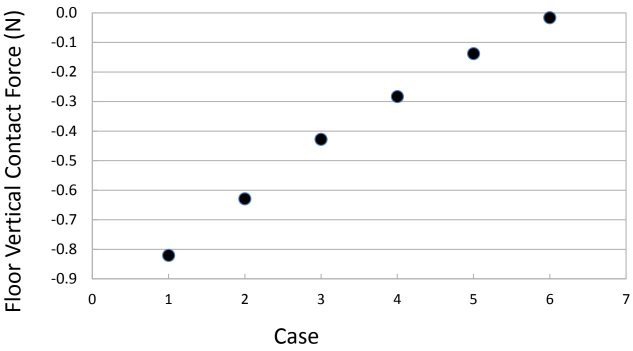

Figure 5: Full Scale Bottom Surface Total Contact Force

Figure 6 compares the pressure drop resulting from the present CFD predictions, to those expected with the Ergun prediction. Similarly, Figure 7 shows the same results in terms of the magnitude of error between STAR-CCM+ predictions and the Ergun correlation. It can be seen that the computational predictions match well prior to fluidization of the bed, with errors being less than 2% under-prediction. As expected, a larger error is seen for Case 6, nearly 12% under-prediction, as

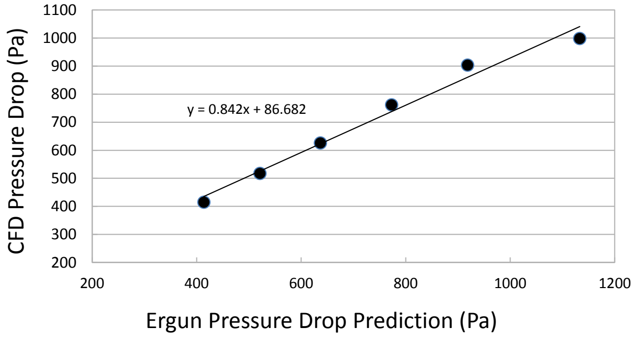

Figure 6: Full Scale CFD Pressure Drop Predictions vs Ergun Predictions

the bed has begun to fluidize and the Ergun prediction is no longer applicable.

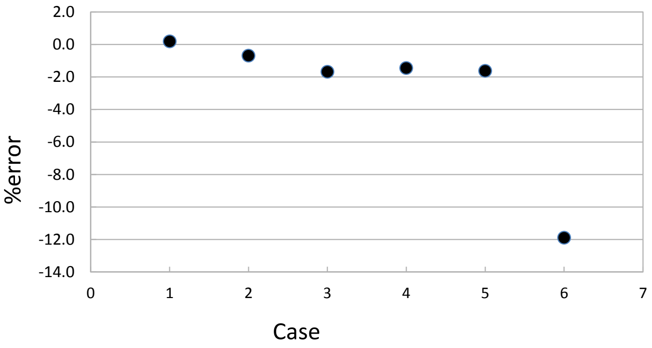

Figure 7: Percent Error in CFD Predictions as Compared to the Ergun Equation

At this point it is worth discussing some of the potential differences between the pressure drops resulting from the CFD simulation, and those predicted by the Ergun equation. The Ergun equation takes into account the bulk, or average, characteristics of the packed bed. For example, the void fraction used in Equations 6 and 7 is the average void fraction for the bed analysed in the current paper. Similarly, the superficial velocity is also an averaged quantity. On the other hand, the computational approach used by STAR-CCM+ accounts for the local variations in the flow characteristics within the bed. As seen in Figure 8, the void fraction (and in effect superficial velocity), tended to vary the greatest across the bed. Nonetheless, the matching can be considered acceptable for the full scale case.

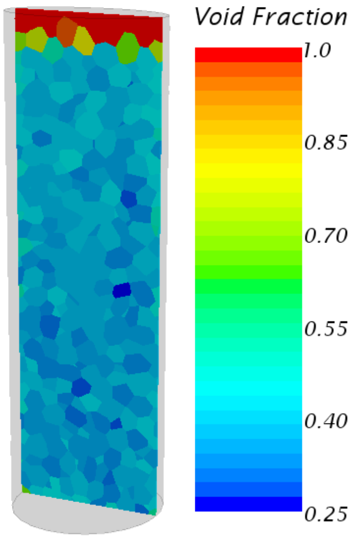

Figure 8: Full Scale Midplane Void Fraction Distribution

SCALED RESULTS

With the full scale results benchmarked, the scaling method discussed above was utilized, with the scaled particle diameter twice that of the full scale model. Hence, the utilized drag coefficient was defined as:

$$C_{d,input} = 2\left(2 * C_{d,scaled} - 1.75\right) \qquad (15)$$

Where $C_{d,scaled}$ is calculated using the Gidaspow correlation based on the scaled geometry and flow characteristics. During the start-up of the simulation, while the residuals were still high, it was necessary to utilize a conditional statement such that $C_{d,input}$ remained positive as the flow developed.

Similar to the full scale cases, Figure 9 highlights the pressure profile along the bed for the scaled Case 1_2X. It can be seen that the results are very similar to those of the full scale case, with a distinct linear profile through the fixed bed, and a reduced pressure drop in the open volume.

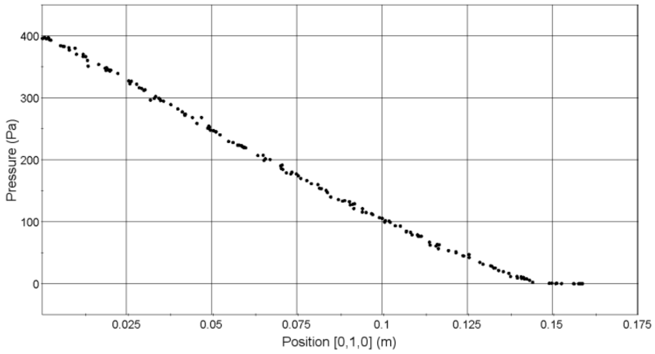

Figure 9: Pressure Profile for Scaled Case 1_2X

Once again examining the contact force on the bottom surface of the domain, one can again identify the point of fluidization for the scaled bed in Figure 10. A monotonic reduction in contact force magnitude is seen as the superficial velocity is increased. For Case 6_2x, the contact force has sufficiently approached zero (-0.028N), suggesting the fluidization of the bed. This is an important result, as the scaling method developed in this paper also results in fluidization velocities which agree with those from full scale analysis. An increase in bed height was also observed for this case on the order of 3mm.

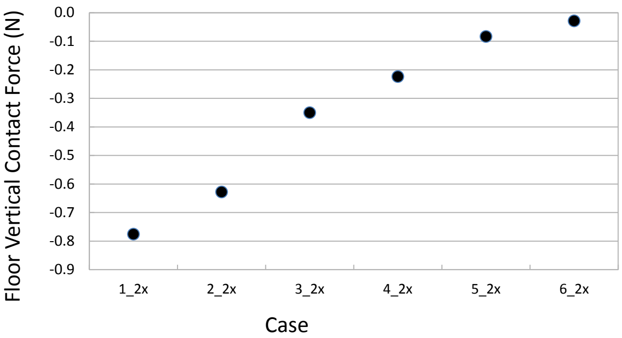

Figure 10: Bottom Surface Contact Force for Scaled Model

Pressure drop predictions from the CFD simulation are compared to those from the Ergun equation in Figure 11. Similarly, percentage errors are reported in Figure 12. From these figures, it is apparent that the scaling method developed here maintains similar accuracies that were observed for the full scale simulation, up to the point of fluidization. For the scaled cases, the computational predictions over predict the values obtained for the full scale model, as predicted by the Ergun equation, by less than 6% for all cases tested. Differences between the full scale simulation and the scaled simulation were less than 8% for all cases prior to fluidization.

The reason for scaling of the DEM particles lies in the fact that the scaled simulation should result in a reduced computational cost. With acceptable accuracies proven, comparisons of solution times can then be made. The simulations discussed in the present paper were carried out on a modern desktop system, with the number of processes set at 4. The full scale cases required 36-48 hours of total CPU time in order to achieve convergence. On the other hand, on the same machine, the scaled cases required 1.5-2 hours of total CPU time to reach convergence. This is an 18-24X speedup, at a cost of less than 10% variation in results. This is a significant improvement, moving from a matter of days to hours.

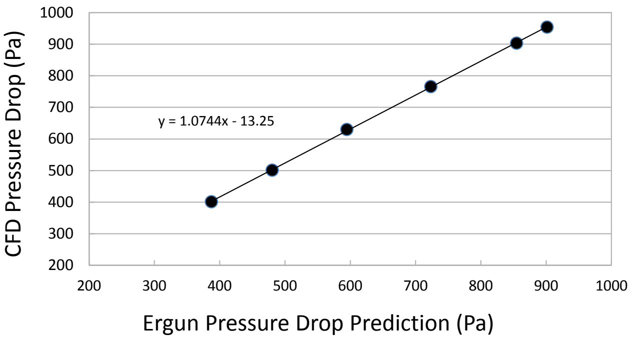

Figure 11: Comparison of Ergun Predictions for the Full Scale Model to the Scaled CFD Model

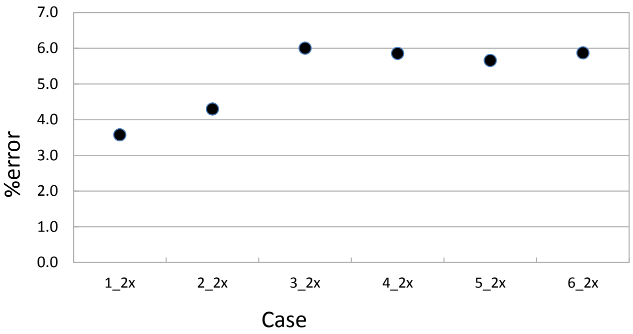

Figure 12: 2X Scale Percent Errors as Compared to the Ergun Predictions

CONCLUSION

This paper has compared the ability of coupled DEM-CFD simulations to accurately predict the pressure drop for the flow through a fixed, packed bed modelled as spherical particles, matching the Ergun equation results within 2%. Additionally, a simple, analytical scaling method was developed in order to take advantage of the reduced computational expense achieved when utilizing larger particles. Through a scaling factor applied to the drag coefficient correlation built into STAR-CCM+, particles with a diameter twice that of the full scale model predicted pressure drops within 6% of the Ergun predictions, and within 8% of the full scale CFD predictions. Additionally, computational costs were significantly reduced, resulting in solution times 18-24 times less than those for the full scale simulation; effectively reducing a potentially multi-day run time to a few hours.

With the accuracy levels adequately maintained through the scaling of the applied drag coefficients in a coupled CFD-DEM, a straight forward approach has been developed allowing for the simulation of packed beds of increased complexity and industrial relevance at reasonable computational costs.

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