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AN INVESTIGATION OF FLUIDIZED BED SCALING LAWS BY DEM SIMULATION

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ABSTRACT

A preliminary investigation of the scaling laws for bubbling fluidized beds was undertaken using Discrete Element Method simulation. Six 2D and two 3D fluidized beds were simulated and compared using bed snapshots and dynamic pressure drop. Beds properly matched by the simplified criteria were in relatively poor agreement; agreement deteriorated further for a large scale change or a particle density mis-match. Simulations matched by the full scaling criteria agreed well at low velocities but deteriorated at higher velocities. The possible reasons for these results are discussed.

INTRODUCTION

For some decades now, hydrodynamic similarity criteria (scaling laws) have been formulated as a possible means of reducing the level of uncertainty associated with the problem of fluidized bed scale-up. However debate regarding the extent of their validity is ongoing and the degree to which these rules are practically applied by industry in process development is unclear. One of the most significant difficulties with evaluating proposed scaling laws for fluidized beds has been gathering reliable evidence for their success or failure based on experimental measurements. Even in well-controlled physical experiments, there is usually some degree of mis-match present in the experimental systems, typically due to difficulties in obtaining real particles perfectly matching in the required particle properties such as sphericity, particle size distribution or density. Unwanted influences not accounted for by the proposed scaling criteria such as electrostatic forces and wall effects may confound experimental results. Additionally, choosing which properties of the bed are to be measured, how they are to be measured, and what analysis method is to be used in comparing the resultant data for scaling law verification is not necessarily a simple matter.

In this study, we have attempted to overcome some of the aforementioned difficulties with experimental validation of fluidized bed scaling criteria by using a Discrete Element Method (DEM) computer simulation of bubbling fluidized beds. Simulation results of six 2D and two 3D fluidized beds were compared for a range of gas velocities and small particle sizes (194 to 388 microns). The beds were set up in accordance with either the simplified or full-set scaling criteria. In order to apply the simplified criteria accurately, a procedure for measuring the minimum fluidization velocity was employed for each particle size in an initial simulation. The effects of density and particle-size mismatches were also considered.

SCALING CRITERIA

Both the "simplified" and "full" scaling criteria for bubbling fluidized beds were chosen for evaluation in this work. The simplified scaling criteria are of practical importance due to the minimal restrictions they impose upon the physical systems to be matched. They can be represented either via the Glicksman *et al* (1) scheme of dimensionless groups (Groups 1) or via the Horio *et al* (2) system of equations (Equations 2a and 2b) with the additional requirement of constant solid to gas density ratio (Group 2c).

$$\frac{gD}{U^2}, \frac{\rho_f}{\rho_s}, \frac{U}{U_{mf}} \tag{1}$$

$$U_2 - U_{mf2} = \sqrt{m}\left(U_1 - U_{mf1}\right) \tag{2a}$$

$$U_{mf2} = \sqrt{m} U_{mf1} \tag{2b}$$

$$\frac{\rho_f}{\rho_s} \tag{2c}$$

In addition to the above requirements, bed geometry, particle sphericity (Φ) and particle size distributions (PSD) should also be maintained similar at the different scales. The full scaling criteria are based on the work of Glicksman (3) and may be represented by the following dimensionless groups:

$$\frac{gD}{U^2}, \frac{\rho_f}{\rho_s}, \frac{\rho_f U d_p}{\mu}, \frac{L}{d_p}, \frac{L_1}{L_2}, \Phi, \text{PSD} \tag{3}$$

DEM SIMULATION

In this work, the simulations used were developed at Monash University from a model made available by Professor M. Horio of Tokyo University of Agriculture and Technology, further details of which can be found in Mikami et al (4). The local averaged Navier-Stokes equations (Anderson and Jackson, (5)) were integrated by the SIMPLE method (Patankar, (6)) employing the staggered grid system for modeling the gas motion. For modeling the particle motion, the Newtonian equations of motion for the individual particles were integrated. Collisions (ie between particles or between particles and a wall) were simulated using Hooke's linear springs and dashpots. For fluid-particle interactions, when the void fraction was less than 0.8, the Ergun equation for packed beds was used; when the void fraction was larger than 0.8, a modified equation of the fluid resistance for a single particle was used. The time-step for calculating particle motion was determined via the following equation after Tsuji et al (7):

$$\Delta t = \frac{1}{5}\sqrt{\frac{(\pi d_p)^3 \rho_s}{6K}} \quad (4)$$

where K is the spring constant (set to 800 N/m). The simulations did not include any applied interparticle forces.

Minimum Fluidizing Velocity

Because the simplified scaling criteria have a velocity parameter U/U_{mf}, for correct scaling by this methodology it is necessary to know the minimum fluidization velocity of each bed material/gas combination *a priori*. As an approximation, a correlation for predicting the U_{mf} (eg 8) can be used, however the experimentally-determined U_{mf} is normally used as the basis for setting up the gas velocity in the scaled beds if conducting a physical experiment. By analogy, it was considered important to base the simulated bed parameters in the present work on the U_{mf} values as determined by simulation.

The minimum fluidizing velocity of each gas-particle combination was determined from simulation using the following procedure. The gas velocity was first increased linearly from 0 to about 1.5 to 2 times the expected U_{mf} (from correlation) over a period of about 0.5 seconds. The velocity was then held constant for a further 0.5 seconds. The gas velocity was then decreased linearly over a period of 14 seconds. Minimum fluidization results were taken from the bed pressure profile generated during the slow velocity decrease stage of the test. It should be noted that this procedure was not necessary for the beds scaled using the full scaling parameters as the minimum fluidizing velocity of the bed is not a required input.

SIMULATION PARAMETERS FOR THE SCALED BEDS

For the two-dimensional study, six different 2D beds were simulated. Particle sizes and densities were chosen to be typical of the Geldart group B materials used in previous physical evaluations of the scaling laws (9). Note that simulated particles were spherical and mono-sized. Pertinent properties of the simulated beds are shown in Table 1.

From Table 1 it can be seen that using Bed 1 as a base scale, Beds 2 and 3 respectively represent a small and a larger scale change following the simplified scaling criteria. Bed 4 is a scale-up of Bed 1 following the simplified scaling criteria but incorporates a mis-matched particle size. Bed 5 is also a scale-up of Bed 1 following the simplified scaling criteria but incorporates a particle density mis-match. Bed 6 is a scale-down of Bed 3 following the full set scaling criteria.

Simulations of the 2D beds were run for 10 seconds (smallest bed) to 25 seconds (largest beds) with bed snapshots obtained every 20th of a second and pressure data sampled at 300 to 500 Hz. Runs were carried out for each bed at up to 6 gas velocities which were appropriately scaled from the superficial gas velocity range of 0.1 to 0.8 m/s used in Bed 1.

Table 1 Simulation parameters for the 2D simulations of scaled and mis-scaled beds

Bed	1	2	3	4	5	6
Particle Diameter, d_p (μm)	194	225	300	300	194	150
Particle Density, ρ_s (kg/m^3)	2650				4100	7485
Gas Density, ρ_f (kg/m^3)	1.17					3.31
Gas Viscosity, μ (Pa.s)	1.85x10^{-5}					
Spring Constant, K (N/m)	800					
Scaling Factor, m	1	1.48	4.42	1.49	1.65	2.21
Minimum Fluidizing Velocity U_{mf} (m/s)	0.056	0.068	0.118	0.118	0.072	0.079
Bed Width, (mm)	16.9	25.0	74.7	25.2	27.9	37.4
Settled Bed Height, (mm)	11.3	16.7	50.1	16.5	18.6	25.1
Vessel Height, (mm)	88.5	129.6	392.4	129.6	146.7	196.2
Number of Particles, N	5046	8214	41583	4620	13824	41583
Number of Fluid Cells (Width x Height)	29 x 76	37 x 96	83 x 218	28 x 72	48 x 126	83 x 218
Time Step, Δt (x10^{-6} s)	2.24	2.79	4.3	4.3	2.78	2.55

Table 2 Simulation parameters for the 3D simulations of full-set scaled beds

Bed	7	8
Particle Diameter, d_p (μm)	194	388
Particle Density, ρ_s (kg/m^3)	2650	935
Gas Density, ρ_f (kg/m^3)	1.17	0.413
Gas Viscosity, μ (Pa.s)	1.85x10^{-5}	1.85x10^{-5}
Spring Constant, K (N/m)	800	800
Scaling Factor, m	1.0 (Basis)	2.0
Bed Width, (mm)	17.0 (Square)	34.1 (Square)
Settled Bed Height, (mm)	11.6	23.2
Vessel Height, (mm)	93.1	186.2
Number of Particles, N	464,640	464,640
Number of Fluid Cells (LxWxH)	22x22x120	22x22x120
Time Step, Δt (s)	2.24x10^{-6}	3.76x10^{-6}
Superficial Gas Velocities, U (m/s)	0.2, 0.6	0.283, 0.849

For the three-dimensional study, two 3D beds, scaled using the full-set scaling criteria were simulated. Due to the computational intensity of modeling beds containing a large number of small particles, only a limited number of runs were performed and these runs were limited in duration to only 3 seconds. Table 2 shows the details of the 3D simulated beds.

RESULTS AND DISCUSSION

For quantitative comparison, the average and standard deviation of the dimensionless bed pressure drop were compared between the scaled beds. The pressure output from the simulation was in Pascals, and for the 2D simulations was non-dimensionalised via the following expression:

$$P^* = \Delta P \frac{A}{Mg} = \frac{6\Delta P(Xd_p)}{\rho_s d_p{}^3 N_p g} \tag{5}$$

where X is the bed width in metres. (For the 3D simulations, the term (Xd_p) in Equation 5 was replaced with X^2 in order to account for the geometry change to 3 dimensions.)

Figure 1 shows the average and standard deviation of dimensionless pressure as a function of superficial gas velocity for Beds 1 to 5. Whilst the dimensionless average bed pressure drops are somewhat similar, the standard deviations of the bed pressures do not coincide particularly well, even for the correctly-scaled beds. This implies that the average bubble dynamics between the simulated beds are not the same. The large scale change (Bed 3) gives the poorest result; the system with deliberately mis-matched particle density (Bed 5) is also in poor agreement. For a qualitative visual comparison, Figure 2 shows typical bed snapshots for each of Beds 1 to 6, at a low and a high superficial gas velocity. At low velocity the simulated beds have a bubbling bed structure with identifiable "bubbles"; at the higher velocity the bubble structure has disappeared and the beds show an open and turbulent structure. Thus at the higher gas velocities the beds are no longer operating in the bubbling regime and it can be argued that under these conditions the scaling criteria are no longer appropriate. However, this argument does not explain the disagreements at low gas velocities (ie U/U_{mf}<5). In contrast to the trend for Beds 1, 2 and 3, van Ommen et al (10), using CFD simulations to investigate scaling criteria, found the agreement for the simplified scaling criteria (ie Equation 1) was better at higher velocity (U/U_{mf} = 5.3) than at lower velocity (U/U_{mf} = 3.4) although they did not achieve full similitude in any of their simulations.

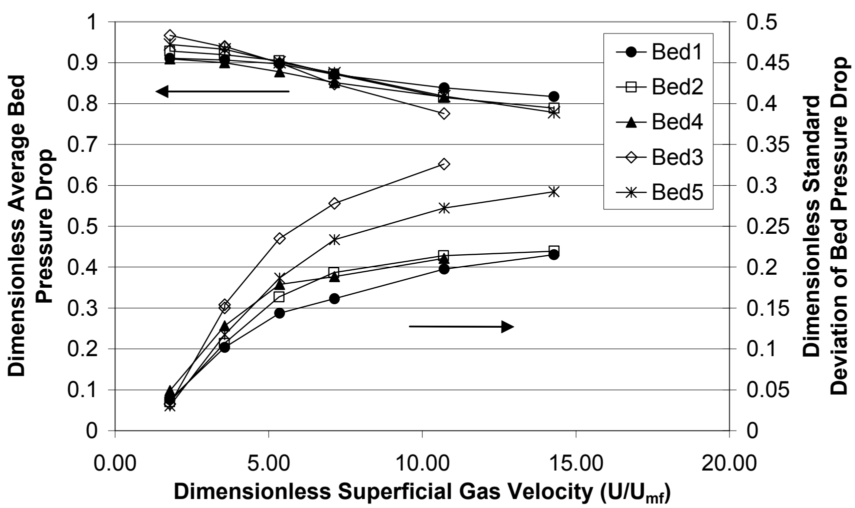
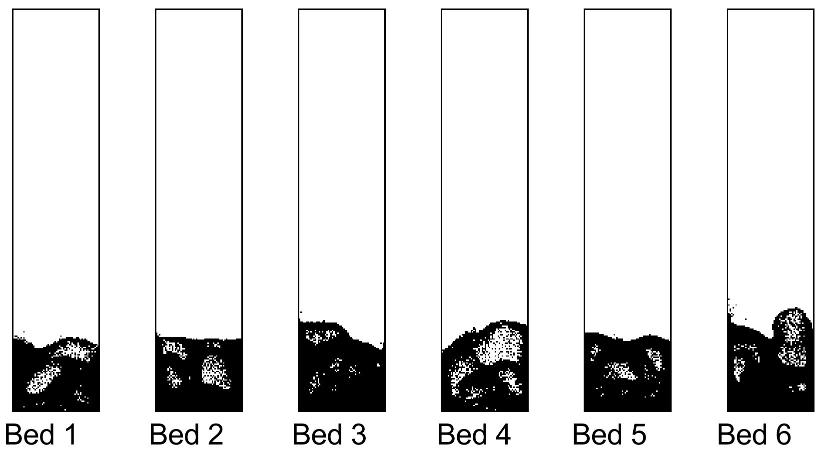
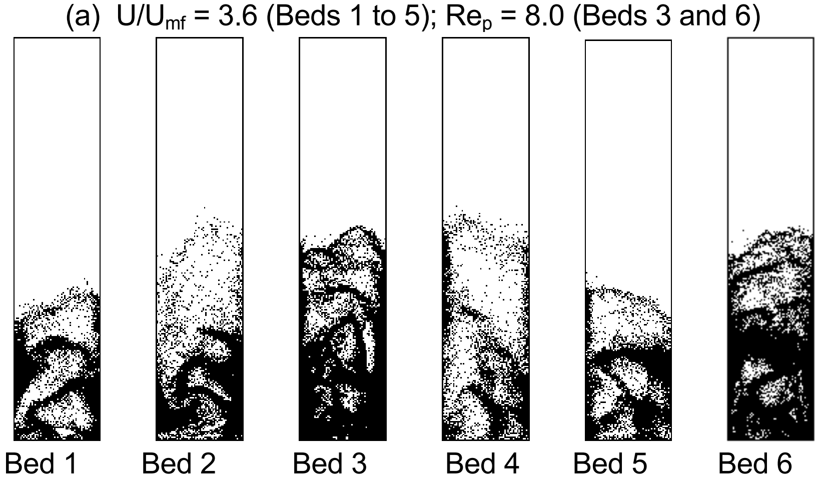


Figure 1 Dimensionless average and standard deviation of bed pressure drop for 2D simulated Beds 1 to 5. (Beds 1 – 3; correct scaling, simplified criteria; Bed 4 = mismatched d_p; Bed 5 = mismatched ρ_s).

Figure 3 shows the average and standard deviation of dimensionless pressure for Beds 3 and 6. Agreement in dimensionless average bed pressure is good at all gas velocities, the standard deviation shows good agreement at low velocity, but diverges at higher velocities. This tends to suggest that the full-set scaling criteria are successful in the 2D simulation for a doubling of size, provided that the bed is in the bubbling regime. Interestingly, in their CFD study, van Ommen et al (10), found the full-set gave worse agreement than simplified set criteria. An additional point of difference between the present 2D DEM simulations involving simplified and full-set scaling criteria relates to the bed *thickness*, which is equal to one particle diameter. For full-set criteria, because the length ratio L/d_p (Equation 3) is maintained constant, bed thickness is scaled along with the other linear bed dimensions. For the simplified criteria, however, particle diameter is chosen based on the minimum fluidization velocity from the dimensionless velocity ratio U/U_{mf} (Equation 1). This implies that the thickness of the 2D beds simulated using simplified criteria is not increased at the same rate as the other bed dimensions in a scaling up.



(a) U/U_{mf} = 3.6 (Beds 1 to 5); Re_p = 8.0 (Beds 3 and 6)



(b) U/U_{mf} = 10.7 (Beds 1 to 5); Re_p = 24.0 (Beds 3 and 6)

Figure 2 Single snapshots of each of the simulated 2D beds showing the typical bed structure at (a) low and (b) high gas velocities.

Table 3 shows the limited dimensionless pressure results from the 3D simulation of beds scaled via full-set criteria. For the conditions studied, the agreements in average and standard deviation of dimensionless bed pressure are reasonable; however not as good as the agreement obtained with the 2D full-set simulations (Beds 3 and 6) at comparable (low) particle Reynolds numbers. One possible reason for the poorer agreement from the 3D simulation may be the relatively short lengths (only 3 seconds) of data available for analysis from each run.

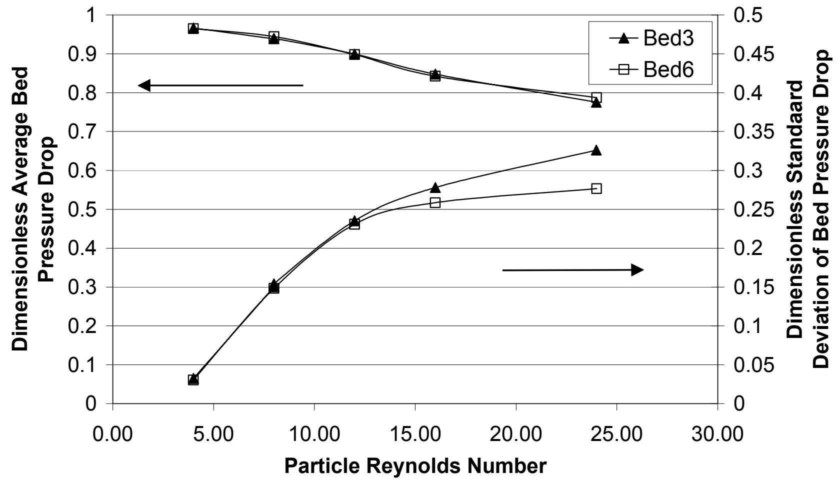


Figure 3 Dimensionless average and standard deviation of bed pressure drop as a function of particle Reynolds number for 2D simulated Beds 3 and 6 (scaled with full-set scaling criteria)

Table 3 Pressure measurement results for the 3D DEM simulation of two beds scaled using the full-set of bubbling bed scaling criteria.

Bed	7	8
Condition 1 (low velocity)		
Particle Reynolds Number	2.45	2.45
Average Bed Pressure (dimensionless)	0.903	0.911
Standard Deviation of Bed Pressure (dimensionless)	0.213	0.239
Condition 2 (high velocity)		
Particle Reynolds Number	7.36	7.35
Average Bed Pressure (dimensionless)	0.841	0.885
Standard Deviation of Bed Pressure (dimensionless)	0.237	0.208

CONCLUSIONS

Some preliminary DEM simulations were undertaken in two and three dimensions with the objective of testing the simplified and full-set scaling criteria for bubbling fluidized beds in a simulated environment. Results for the 2D simulations, in the form of pressure data and bed snapshots, indicated that the simplified criteria performed poorly in all cases, especially for a large scale change or a deliberate particle density mis-match. The full-set of scaling criteria performed well at low velocity for the scale change investigated, but agreement deteriorated at high velocity, most likely due to the simulated beds no longer operating in the bubbling regime. Results from two 3D simulations of beds matched with the full-set scaling parameters did not agree as well as those at low velocity from the 2D study; this may have been due to the limited length of data available from the 3D simulations. Further 3D simulation work on both simplified and full-set scaling criteria is still required.

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NOTATION

A	Bed cross-sectional area (m^2)	Re_p	Particle Reynolds number
D	Bed diameter (m)	U	Superficial gas velocity (m/s)
d_p	Particle diameter (μm)	U_{mf}	Minimum fluidization velocity (m/s)
g	Acceleration due to gravity (m/s^2)	X	Bed width (m or mm)
K	Spring constant (800 N/m)	Δt	Simulation time step (s)
L	Characteristic length (m)	ΔP	Bed pressure drop (Pa)
m	Linear scaling factor	μ	Fluid viscosity (kg/ms)
M	Bed mass (kg)	Φ	Particle sphericity
N_p	Number of particles	ρ_s	Particle density (kg/m^3)
P*	Dimensionless pressure	ρ_f	Fluid density (kg/m^3)

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