UNIVERSITYOF BIRMINGHAM

A DEM investigation of transitional behaviour in gas-fluidised beds

Thornton, Colin; Yang, Fang; Seville, Jonathan

Document Version
Publisher's PDF, also known as Version of record

Publisher Rights Statement:
Eligibility for repository : checked 11/11/2014

A DEM investigation of transitional behaviour in gas-fluidised beds

Colin Thornton *, Fang Yang, Jonathan Seville [1]

School of Chemical Engineering, University of Birmingham, Birmingham B15 2TT, UK

A R T I C L E   I N F O

A B S T R A C T

Using DEM simulations, the paper examines the different types of behaviour as the gas velocity is increased to cover the complete range from fixed bed to homogeneous expansion, bubbling, turbulent and fast fluidisation. The paper highlights the transitions between the various regimes. At minimum fluidisation velocity, U_{mf}, the structure of the bed is isostatic. When the gas velocity U is increased the system immediately breaks up into large clusters of contacting particles which gradually disintegrate with further increases in gas velocity until, at minimum bubbling velocity, U_{mb}, the first bubbles start to appear. Conventionally, the regime $U_{mf} < U < U_{mb}$ is referred to as homogeneous expansion. However, it is shown that the expansion is not homogeneous. Above U_{mb}, the amplitude of the pressure drop fluctuations increases to a maximum when $U = U_c$, which marks the transition from bubbling to turbulent behaviour. The simulations also show that in the turbulent regime the average pressure drop increases with increasing gas velocity. This aspect appears not to have been reported previously in the literature. Finally, when $U > U_k$, corresponding to "fast fluidisation", the particle system behaves as a granular gas. A new criterion is suggested to define the transition from turbulent fluidisation to fast fluidisation, defined by U_k.

1. Introduction

Gas-fluidised beds have been extensively studied in academia and widely used in industry. When examined at the macro-scale, fluidised beds may appear to behave like a solid, a liquid or a gas, depending on the magnitude of the applied superficial gas velocity. These "phase transitions" are important since the fundamental rate parameters for reactor design and operation change in accordance with the flow regimes of fluidisation. One of the attractions of the Discrete Element Method (DEM) is that it can model all three different phases. To account for the interstitial gas, following Tsuji et al. [1], a combined Lagrangian–Eulerian approach is used by combining the use of DEM for the particle phase with CFD modelling of the gas phase. Complete details of the methodology are provided by Kafui et al. [2]. Using DEM–CFD simulations, the paper examines the different types of behaviour as the gas velocity is increased to cover the complete range from fixed bed to homogeneous expansion, bubbling, turbulent and fast fluidisation. This is the first DEM–CFD study of gas-fluidised beds to cover the complete range of applied gas velocities.

2. Simulation details

Two dimensional DEM–CFD simulations were performed using a container of height = 15.5 mm, and width = 2 mm. The whole container is divided into small computational fluid cells, the size of which is $5d_p \times 5d_p$, where d_p is the mean particle diameter. The bed width corresponds to 40 times the mean particle diameter. The input parameters used for the gas phase and the particle phase are given in Tables 1 and 2, respectively. The mean particle diameter is 50 μm, corresponding to Geldart Group A type particles, for which van der Waals forces significantly affect the particle interactions. The particle system is the same as that used by Yang et al. [3] who examined the effect of surface energy on the transition from fixed bed to bubbling bed. However, in this paper, the particles are modelled as non-adhesive, frictional elastic spheres for which the normal contact force model is that of Hertz, see Johnson [4] and the tangential contact force model is defined by the theory of Mindlin and Deresiewicz [5], see also Thornton and Yin [6], and Thornton et al. [7].

In these 2D simulations, all the particles were initially randomly generated as a granular gas (no contacts) within the 2 mm wide container. The centres of all particles were located in the same plane and subsequent out-of-plane motion was suppressed. A vertical gravity field was introduced in order to create a pluvially deposited bed of particles. The initial bed height was 6.54 mm and the initial voidage was 0.459. During the simulations the pressure is recorded for each fluid

* Corresponding author.
  E-mail address: c.thornton@bham.ac.uk (C. Thornton).
[1] Present address: Department of Chemical & Process Engineering, University of Surrey, Guildford, Surrey GU2 7XH, UK.

Table 1
Gas phase input parameters.

Average gas molar mass	2.88E−2 kg/mol
Gas viscosity	1.8E−5 kg/m·s
Gas density	1.1979 kg/m³
Gas pressure (atmospheric)	101.3 kPa
Gas temperature	293 K

Table 2
Particle phase input parameters.

Number of particles	5000
Mean particle diameter	50 μm
Particle sizes	45, 47.5, 50, 52.5, 55 μm
Young's modulus	700 MPa
Particle density	2500 kg/m³
Poisson's ratio	0.33
Friction coefficient	0.30

cell and the pressure difference between the bottom layer of cells and the layer of cells at the top of the container is taken as the pressure drop across the bed ΔP. The normalised bed pressure drop ΔP* is defined as

$$\Delta P^* = \frac{\Delta P}{gM/A} \tag{1}$$

where, neglecting the negligible gas density,

$$M = \frac{\pi}{6}\rho_p \sum d_p^3 \tag{2}$$

and M is the total mass of particles, ρ_p and d_p are the solid density and diameter of a particle, g is the acceleration due to gravity and A is the cross sectional area of the bed. In the 2D simulations, the depth of the bed is simply considered as one mean particle diameter. Based on

this simplification, for the 2 mm wide bed, $A = 1 \cdot 10^{-7}$ m² and the bed weight per unit area is 81.15 Pa. The overall average voidage of the bed is defined as

$$\varepsilon = 1 - \frac{\sum_{i=1}^{N} V_i}{AH} \tag{3}$$

where V_i is the volume of particle i. The bed height H is determined in the following way. First, the fluidised bed is divided into eight vertical columns. For each column, the topmost particle is identified and the highest fluid cell in which the topmost particle resides is recorded at the same time. The average height for each column is computed by accumulating all of the heights of particles in each of the highest fluid cells and then calculating the average value. Finally, with the mass of the particles in each highest cell as the weighting parameter, the whole bed height is then calculated by taking the average of all the average column heights.

An initial uniform gas flow U = 0.0003 m/s was introduced into the bed from the bottom row of computational fluid cells. The pressure drop across the bed was obtained as the time-averaged difference between the average pressure in the bottom and top rows of fluid cells. This was repeated for a range of gas velocities incremented in relatively small steps up to 1.2 m/s. With increasing gas velocity, bed expansion increases and particles are transported higher. Consequently, in the turbulent regime simulations, the height of the container and the corresponding fluid computational domain were adjusted to ensure that particles did not reach the top boundary of the container.

3. Results and discussion

Fig. 1 shows how the average void fraction of the bed changes with increasing superficial gas velocity. There are clearly three regimes. At low gas velocities the void fraction does not change. This corresponds to the fixed bed regime that exhibits solid-like behaviour. At high gas velocities, as the void fraction ε → 1 the behaviour is gas-like corresponding to fast fluidisation, as in the riser of a circulating fluidised bed. Between these two regimes the bed behaves like a liquid but there is no indication in the figure to distinguish between the bubbling
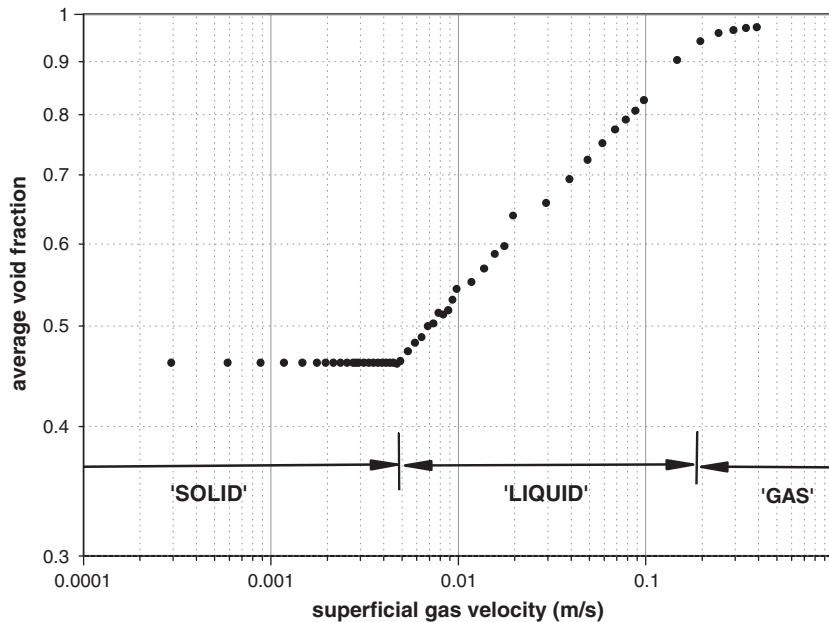

Fig. 1. Variation of the average bed void fraction with increasing superficial gas velocity.
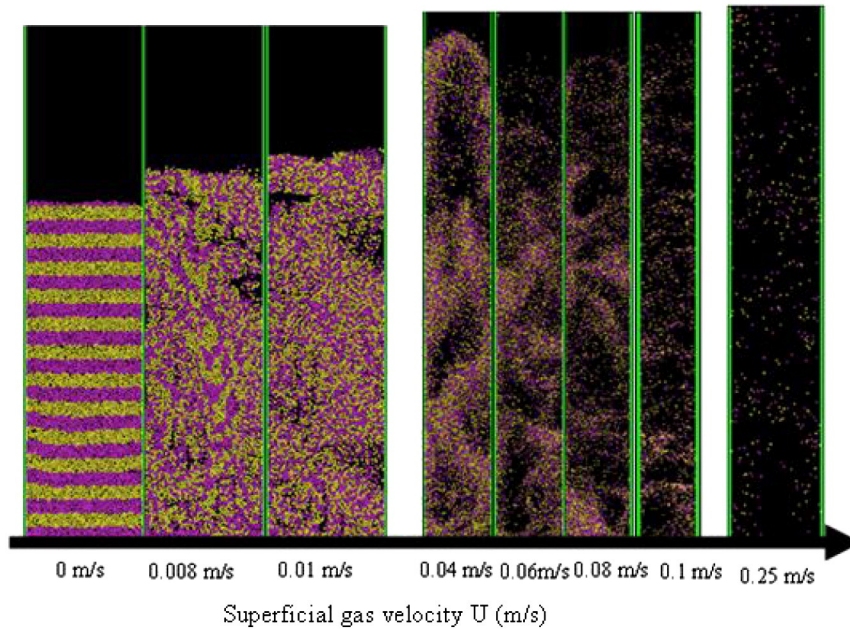
Fig. 2. Typical particle configurations for different superficial gas velocities.

and turbulent subregimes. Fig. 2 shows typical particle configurations at different superficial gas velocities. The figure illustrates that in the liquid-like regime there are three subregimes corresponding to homogeneous expansion, bubbling fluidisation and turbulent fluidisation. The transitions between these subregimes will be discussed below.

3.1. The transition from fixed to bubbling bed

Conventionally [8] the point when the average pressure drop first becomes equal to the bed weight divided by the cross-sectional area of the bed is defined as 'minimum fluidisation' and the gas velocity at which this occurs is denoted as U_{mf}. Above U_{mf} the pressure drop remains constant and bed expansion occurs. In Fig. 3, the average pressure drop is normalised by dividing by the bed weight per unit area. From the figure, $U_{mf} = 0.0048$ m/s, which is in reasonable agreement with the value of 0.0041 m/s predicted using the Ergun correlation [9].

Superimposed in Fig. 3 is the number of inter-particle contacts normalised by the initial number of contacts when the bed had been deposited. It can be seen that some contacts were broken, without any
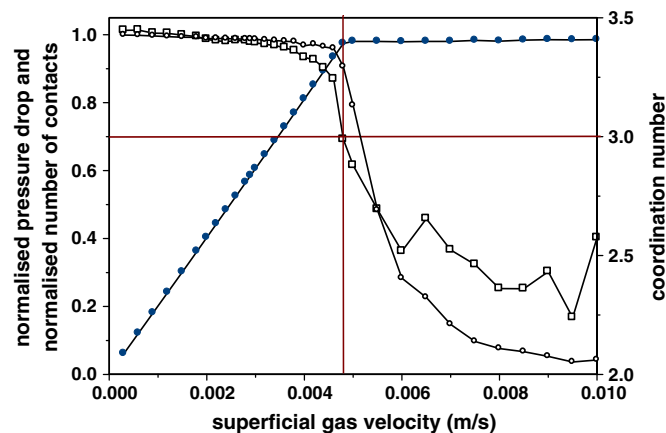
significant change in voidage/bed height, prior to minimum fluidisation and that, above U_{mf}, the average number of contacts decreased at a decreasing rate until an asymptotic value of about 5% of the initial number of contacts was reached when $U = 0.01$ m/s. Also superimposed in the figure is the mechanical coordination number Z_m defined by

$$Z_m = \frac{(2C - N_1)}{(N - N_1 - N_0)} \qquad (4)$$

where C is the number of contacts and N is the number of particles, N_1 is the number of particles with only one contact and N_0 is the number of particles with no contacts, see Yang et al. [3]. From the figure it can be seen that, when $U = U_{mf}$, $Z_m = 3$. This corresponds to an isostatic state. When $Z_m > 3$ the system is redundant, i.e. there are more contacts than necessary to ensure stability. When $Z_m < 3$ there are not enough contacts for stability and the system becomes a mechanism.

Fig. 4 shows the expansion of the bed as the gas velocity is increased to 0.01 m/s. From examination of video sequences of the simulations it was observed that the first bubble eruption at the bed surface occurred when $U = 0.01$ m/s. Consequently we take the minimum bubbling velocity to be $U_{mb} = 0.01$ m/s $= 2.08 U_{mf}$.

The gas velocity range $U_{mf} < U < U_{mb}$ is conventionally known as the homogeneous expansion regime. Fig. 5 shows snapshots to illustrate the evolution of the structure of the bed at the start of the bed expansion. In each snapshot, the three columns show (i) the six largest cluster sizes in the system (left column), (ii) the fines consisting of singlets, doublets and triplets (centre column) and (iii) the spatial distribution of interparticle contacts (right column). Note that clusters of intermediate sizes are not shown. It can be seen that the number of contacts decreases sharply for 0.0048 m/s < U < 0.006 m/s with a corresponding sharp increase in the number of fines. The figure clearly shows the degradation of large clusters, the increase in fines production and the corresponding loss of contacts as the gas velocity increases.

From Fig. 5 it is also clear that, at least at the start of the 'homogeneous expansion' regime the bed is not in fact homogeneous. It is therefore suggested that the so-called homogeneous expansion regime is actually a transition regime. At U_{mf} the bed is at an isostatic state corresponding to 'incipient fluidisation' [10] which is the start of a transition from solid-like to fluid-like behaviour and that only when the contact
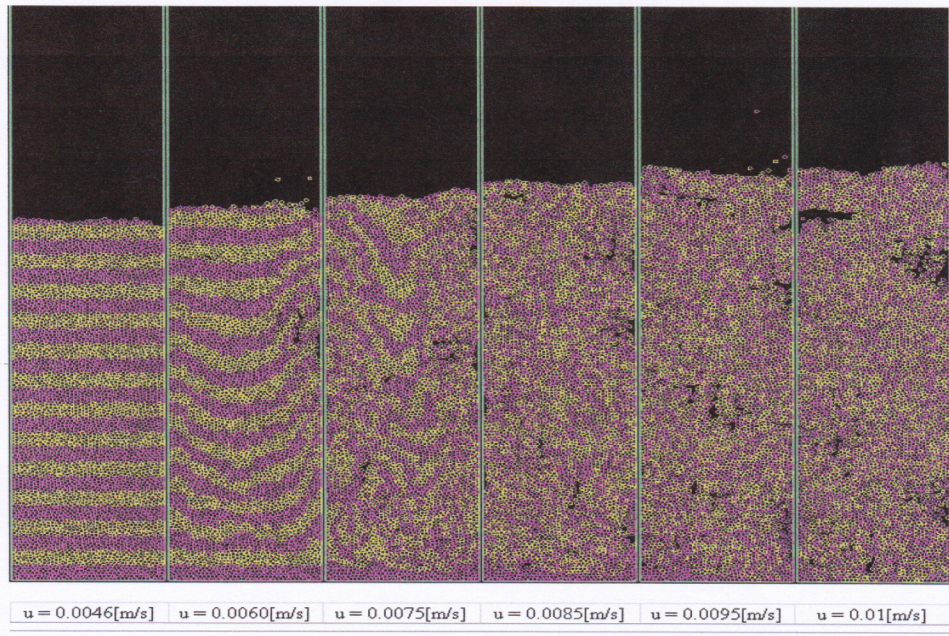

Fig. 3. Normalised pressure drop (solid circles), normalised number of contacts (open circles) and mechanical coordination number (open squares).

| u = 0.0046[m/s] | u = 0.0060[m/s] | u = 0.0075[m/s] | u = 0.0085[m/s] | u = 0.0095[m/s] | u = 0.01[m/s] |

Fig. 4. Bed expansion with increasing gas velocity.

number reaches a small asymptotic value is the bed 'fully fluidised' and bubbling can then occur.

3.2. The transition from bubbling bed to turbulent bed

Above U_{mb} bubbling occurs, with the size of the bubbles increasing with increase in gas velocity. As a consequence of bubble eruption at the top of the bed, the amplitude of the pressure drop fluctuations also increases with increase in gas velocity. In this bubbling regime both bubble splitting and bubble coalescence occur. When bubble splitting exceeds bubble coalescence the mean bubble size decreases and this leads to a decrease in the amplitude of the pressure drop fluctuations. This is illustrated in Fig. 6. Fig. 7 shows how the standard deviation of the normalised pressure drop varies with superficial gas velocity. It can be seen that the standard deviation of the pressure drop increases to a maximum value and then reduces at a decreasing rate to an asymptotic value.

Yerushalmi et al. [11] and Yerushalmi and Cankurt [12] suggested that the gas velocity U_c at which the standard deviation of the pressure drop reaches a maximum value indicates the beginning of a transition to turbulent fluidisation. They also suggested that the gas velocity U_k at which the standard deviation of the pressure drop levels off at some low value indicates the end of the transition. However, subsequent researchers have adopted U_c as the start of the turbulent regime and U_k as the end of the turbulent regime and the transition to fast fluidization [13]. From Fig. 7 we deduce that $U_c = 0.085$ m/s but it is clear from the figure that the above definition of U_k is ambiguous. It is also noted that in the turbulent regime $(U > U_c)$ the average pressure drop increases with increasing gas velocity. This aspect appears not to have been reported previously in the literature.

Figs. 8 and 9 show typical visualisations of the particle configuration, the gas velocity field and the particle velocity field in the bubbling regime and the turbulent regimes respectively. As can be seen in the figures, a distinction between the two regimes is that, in the bubbling regime the 'discontinuous' gas phase, in the form of bubbles, changes
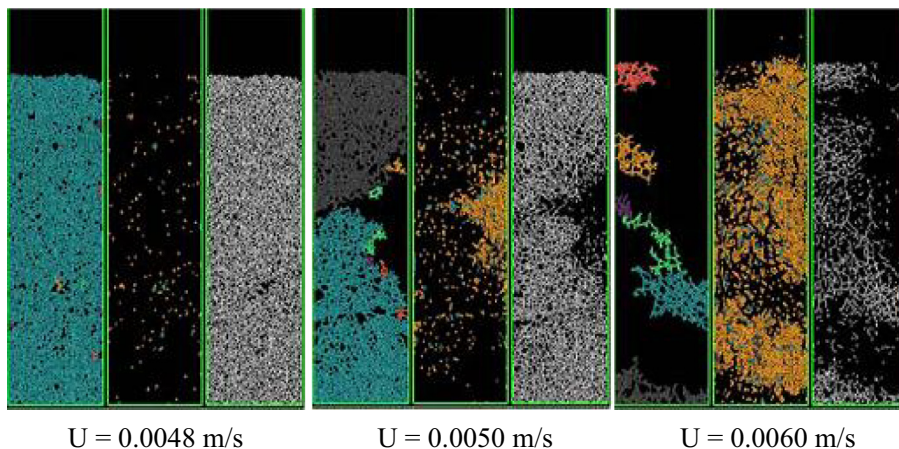

U = 0.0048 m/s   U = 0.0050 m/s   U = 0.0060 m/s

Fig. 5. Cluster visualisation at the start of the 'homogeneous expansion' regime.
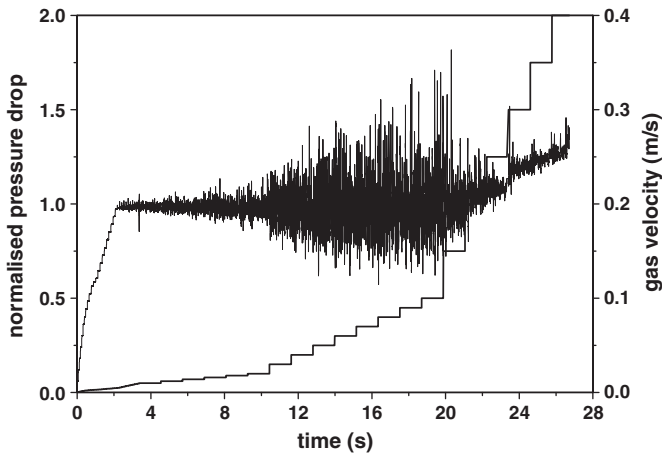
Fig. 6. Non- averaged pressure drop fluctuations.

to a continuous gas phase in the turbulent regime. Correspondingly, the solid phase changes from continuous to discontinuous when $U > U_c$.

3.3. Bed expansion

The voidage data shown in Fig. 1 for the "liquid" regime indicates power law behaviour. This is confirmed in Fig. 10 in which the void fraction and the gas velocity have been normalised by the corresponding values at minimum fluidisation, i.e. $\varepsilon_{mf} = 0.459$ and $U_{mf} = 0.0048$ m/s respectively. From the best fit line we obtain the following relationship.

$$\frac{U}{U_{mf}} = \left(\frac{\varepsilon}{\varepsilon_{mf}}\right)^{5.2} \tag{5}$$

From which we obtain

$$U = 0.275\varepsilon^{5.2} . \tag{6}$$

Eq. (6) implies that when $\varepsilon = 1$ the gas velocity of 0.275 m/s corresponds to the free-fall terminal velocity, U_t, of an isolated sphere in an infinite fluid [10]. Using a single average-sized sphere, $d_p = 50$ µm,

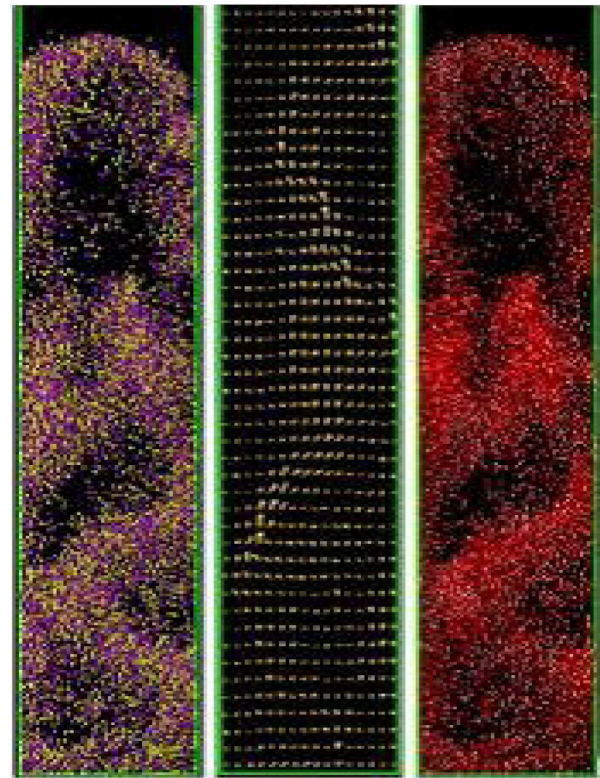**Fig. 8.** Particle configuration (left), gas velocities (centre) and particle velocities (right) in the bubbling regime (U = 0.04 m/s).

and atmospheric gas with the initial gas velocity set to zero, the gravity driven free-fall of an isolated particle was simulated and the terminal velocity was found to be 0.3 m/s. The data point corresponding to $U_t = 0.3$ m/s is indicated in Fig. 10. It is noted that as the gas velocity approaches U_t the data deviate from the power law relationship. It is suggested that the point at which data first starts to deviate from the power law is taken to indicate the transition from turbulent behaviour to fast fluidisation, U_k. From Fig. 10, $U_k = 0.2$ m/s.
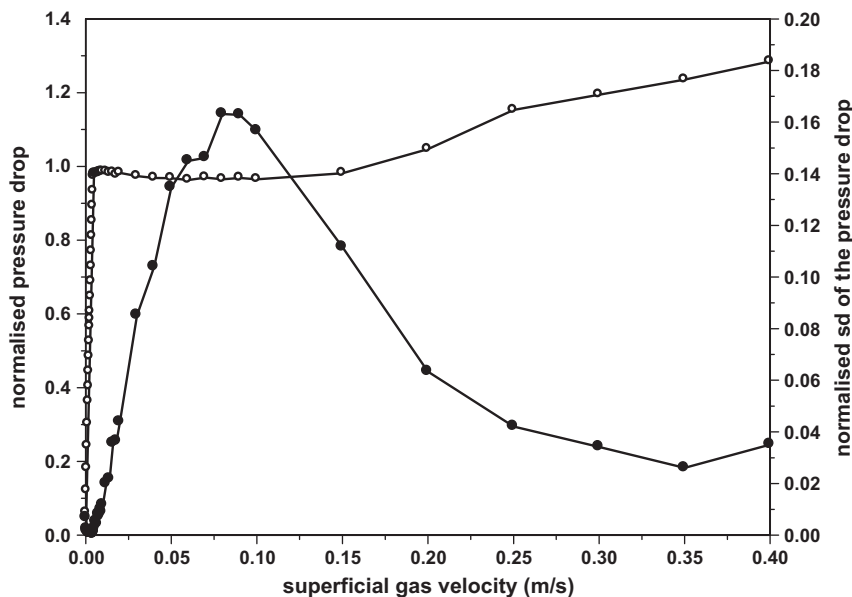

Fig. 7. Variation of the standard deviation (sd) of the normalised pressure drop with superficial gas velocity.
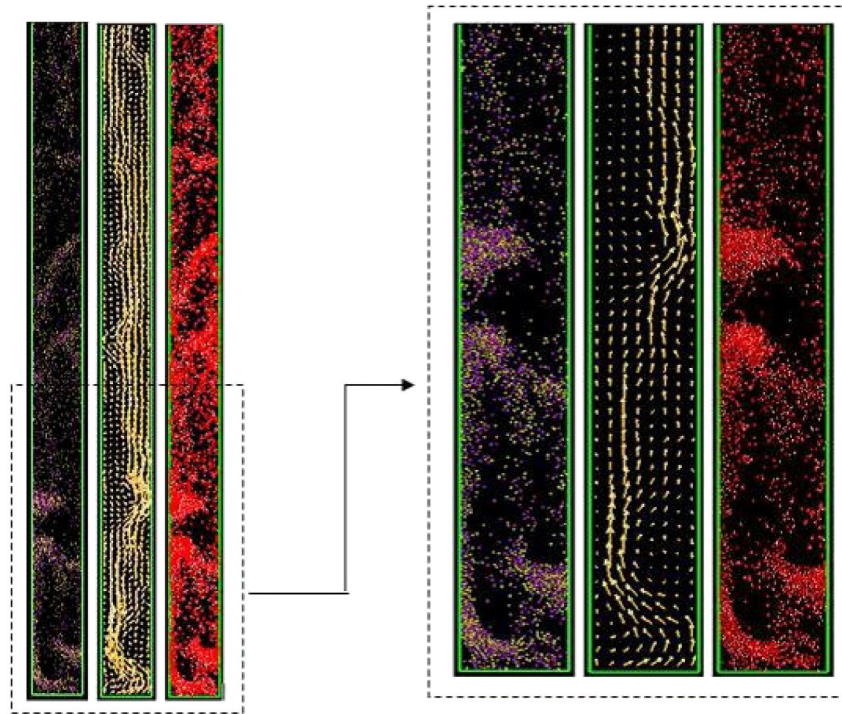
Fig. 9. Particle configuration (left), gas velocities (centre) and particle velocities (right) in the turbulent regime (U = 0.15 m/s).

4. Summary

A combined DEM–CFD code has been used to study the fluidised behaviour of a 2D cohesionless fine particle bed for a wide range of superficial gas velocities in order to identify the different behavioural regimes. From the result obtained from the simulations the following conclusions are drawn:

- For the particle size distribution and initial bed voidage used, the point of minimum fluidization is unambiguous and $U_{mf} = 0.0048$ m/s, in reasonable agreement with the prediction of $U_{mf} = 0.0041$ m/s obtained using the empirical correlation due to Ergun [9].

- In spite of the subjective nature of visual observations, including video sequences, the authors conclude that $U_{mb} = 0.01$ m/s, corresponding to $U_{mb} = 2.08$ U_{mf}. In agreement with conventional wisdom, it is considered that the transition to turbulent flow occurs when the standard deviation of the pressure drop reaches a maximum value and therefore, for the simulations reported, $U_c = 0.085$ m/s = 17.7 U_{mf}.
- It is suggested that the transition from turbulent to fast fluidisation is given by the point at which the void fraction first starts to deviate from the power law behaviour and hence $U_k = 0.2$ m/s = 41.7 U_{mf}.
- A summary of the values of all the transitional gas velocities and their relationship to U_{mf} and U_t is provided in Table 3.

Although particles of the sizes used in these simulations would, in reality, be adhesive due to van der Waals forces, it has been demonstrated [3] that the effect of surface energy is negligible once bubbling occurs. Consequently we expect that our findings are also applicable to adhesive particle systems except for the magnitude of U_{mb}, see Yang et al. [3] for further details.

Finally, when considering the actual, rather than the relative, magnitudes of the gas velocities at the various transitions it would be expected that the values would be slightly different in 3D.
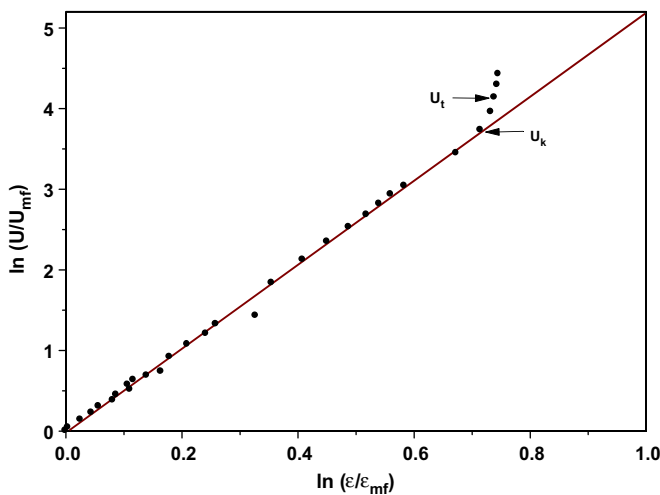
Fig. 10. Power law fit to the data in the bubbling and turbulent regimes. The point at which data first starts to deviate from the power law is taken to indicate the transition from turbulent behaviour to fast fluidisation denoted by U_k. Also shown in the figure is the point corresponding to U_t, the terminal velocity of a single average sized sphere.

Table 3
Summary of transitional gas velocities.

	U (m/s)	U/U_{mf}	U/U_t
U_{mf}	0.0048	1.0	0.016
U_{mb}	0.01	2.08	0.033
U_c	0.085	17.7	0.283
U_k	0.2	41.7	0.667
U_t	0.3	62.5	1.0

References

[1] Y. Tsuji, T. Kawaguchi, T. Tanaka, Discrete particle simulation of two-dimensional fluidized bed, Powder Technol. 77 (1993) 79–87.

[2] K.D. Kafui, C. Thornton, M.J. Adams, Discrete particle-continuum fluid modeling of gas-solid fluidized beds, Chem. Eng. Sci. 57 (2002) 2394–2410.

[3] F. Yang, C. Thornton, J.P.K. Seville, Effect of surface energy on the transition from fixed to bubbling gas-fluidised beds, Chem. Eng. Sci. 90 (2013) 119–129.

[4] K.L. Johnson, Contact Mechanics, Cambridge University Press, 1985.

[5] R.D. Mindlin, H. Deresiewicz, Elastic spheres in contact under varying oblique force, Trans. ASME J. Appl. Mech. 20 (1953) 327–344.

[6] C. Thornton, K.K. Yin, Impact of elastic spheres with and without adhesion, Powder Technol. 65 (1991) 113–123.

[7] C. Thornton, S.J. Cummins, P.W. Cleary, An investigation of the comparative behaviour of alternative contact force models during elastic collisions, Powder Technol. 210 (2011) 189–197.

[8] D. Geldart, Gas Fluidisation Technology, Wiley, 1986.

[9] S. Ergun, Fluid flow through packed columns, Chem. Eng. Prog. 48 (1952) 89–94.

[10] J.F. Davidson, D. Harrison, Fluidised Particles, Cambridge University Press, 1963.

[11] J. Yerushalmi, N.T. Cankurt, D. Gerldart, B. Liss, Flow regimes in vertical gas–solid contact systems, AIChE Symp. Ser. 174 (1978) 1–12.

[12] J. Yerushalmi, N.T. Cankurt, Further studies of the regimes of fluidization, Powder Technol. 24 (1979) 187–205.

[13] H.T. Bi, N. Ellis, I.A. Abba, J.R. Grace, A state-of-the-art review of gas–solid turbulent fluidization, Chem. Eng. Sci. 55 (2000) 4789–4825.