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Eulerian Simulations of Bubbling Behaviour in Gas-Solid Fluidised Beds

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Abstract

In literature little attempt has been made to verify experimentally Eulerian-Eulerian gas-solid model simulations of bubbling fluidised beds with existing correlations for bubble size or bubble velocity. In the present study, a CFD model for a free bubbling fluidised bed was implemented in the commercial code CFX of AEA Technology. This CFD model is based on a two fluid model including the kinetic theory of granular flow. Simulations of the bubble behaviour in fluidised beds at different superficial gas velocities and at different column diameters are compared to the Darton et al. (1977) equation for the bubble diameter versus the height in the column and to the Hilligardt and Werther (1986) equation, corrected for the two dimensional geometry using the bubble rise velocity correlation of Pyle and Harrison (1967). It is shown that the predicted bubble sizes are in agreement with the Darton et al. (1977) bubble size equation. Comparison of the predicted bubble velocity with the Hilligardt and Werther (1986) equation shows a deviation for the velocity of smaller bubbles. To explain this, the predicted bubbles are divided into two bubble classes : bubbles that have either coalesced, broken-up or have touched the wall, and bubbles without these occurrences. The bubbles of this second class are in agreement with the Hilligardt and Werther (1986) equation. Fit parameters of Hilligardt and Werther (1986) are compared to the fit parameters obtained in this work. It is shown that coalescence, break-up, and direct wall interactions are very important effects, often dominating the dynamic bubble behaviour, but these effects are not accounted for by the Hilligardt and Werther (1986) equation.

Introduction

Fluidised multiphase reactors are of increasing importance in nowadays chemical industries, even though their hydrodynamic behaviour is complex and not yet fully understood. Especially the scale-up from laboratory towards industrial equipment is a problem. For example, equations describing the bubble behaviour in gas-solid fluidised beds are (semi) empirical and often determined under laboratory conditions. For that reason there is little unifying theory describing the bubble behaviour in fluidised beds.

Computational fluid dynamics (CFD) is becoming more and more an engineering tool to predict flows in various types of apparatus on industrial scale. Although the tools for applying single phase flow CFD are widely available, application of multiphase CFD is however still complicated from both a physical and a numerical point of view. Moreover, experimental validation of multiphase CFD models is still in its infancy because simulations are time consuming and reliable predictions of average flows in large scale equipment are therefore not readily obtained. Almost all the work on the simulation of gas-solid fluidised beds is limited to a qualitative (visual) comparison of simulated bubble shapes or bubble sizes with pictures of bubbles obtained from single orifice experiments of bubble formation and bubble growth (e.g., Kuipers et al., 1991). Obvious reasons for this are the already mentioned time consuming character of the simulations as well as the lack of reliable measurements for validating the calculated predictions. Moreover the research efforts of most groups working in this field are aimed at development of still more detailed CFD models for two phase flow, while little attention is paid to the evaluation of the simulation results from an engineering point of view. This is strange, because at the one hand, nowadays the computational power of modern computers is increasing considerably, enabling the simulation of many bubbles in relatively large scale equipment; at the other hand, in the classical fluidisation literature an abundance of data is available in the many (semi) empirical correlations that relate bubble sizes and rise velocities in single and multiple bubble beds to fluidisation conditions.

Recently for Geldart group A powders, Ferschneider and Mège (1996) have used a Eulerian CFD model for the simulation of free bubbling fluidised beds, for one fluidisation condition, showing the bubble sizes and bed expansion. They concluded that although the model predicts the bubble sizes throughout the bed correctly for *one* specific fluidisation condition, the model is *not* suitable to predict the bed expansion of this type of particles. The purpose of the work presented in this paper is to quantitatively compare the Eulerian-Eulerian simulation of bubble sizes and rise velocities in fluidised beds with Geldart group B particles, at different fluidisation conditions, with predictions by generally accepted and applied equations that can be found throughout the litera-

ture. This will provide insight into the validity of this type of CFD codes used in the simulations of free bubbling fluidised beds. If these codes appear to be applicable, they can be used to generate engineering correlations to be used in the design of bubbling fluidised bed reactors.

Gas-solid multiphase model

In spite of the increasing computational power, the number of particles in gas-solid flow in large scale equipment is still much too large to handle each particle separately. Simulating each particle separately is called a Lagrangian method, which can be used to study microscopic properties of fluidised beds (Tsuji et al., 1993). The CFD model used in this work, however, is based on a two fluid model (TFM) extended with the kinetic theory of granular flow as derived from the kinetic theory of gases (Chapman and Cowling, 1970). In a TFM both phases are considered to be continuous and fully interpenetrating. The TFM has first been proposed by Anderson and Jackson (1967) and Pritchett et al. (1978). These firstly proposed models have zero gas and solids viscosities. Physical behaviour dominated by the drag between the solids phase and the gas phase, like the formation of bubbles at a single orifice, is successfully predicted by these models. To overcome the deficiency of these inviscid models, for instance not being able to describe the forces on tubes, a solids viscosity was added to the model by Jackson (1985). Unfortunately realistic physical values for this solids viscosity as well as for the solids stresses were not known.

Jenkins and Savage (1983), Lun et al. (1984), and Ding and Gidaspow (1990) described the solids phase as a non-interstitial fluid. This approach is based on the kinetic theory of dense gases, as presented by Chapman and Cowling (1970). In this approach the usual thermodynamic temperature is replaced by the granular flow temperature. The solids viscosity and stress are a function of this granular temperature, which varies with time and position in the fluidised bed.

Continuity and momentum equations

Different physical TFM models exist in literature, and have been described and compared to each other by Boemer et al. (1995). The most promising set of equations in the sense of fast numerical convergence and accurate physical results is used in this work.

The well-known continuity equation, or mass balance for phase i (gas or solid) reads :

$$\frac{\partial}{\partial t}(\epsilon_i \rho_i) + \nabla \cdot (\epsilon_i \rho_i \mathbf{v}_i) = 0 \qquad (1)$$

$$\epsilon_g + \epsilon_s = 1 \qquad (2)$$

where ϵ is the volume fraction of each phase, $\mathbf{v}$ the velocity, and ρ the density. Mass exchange between the phases, e.g. due to reaction or combustion, is not considered.

The momentum balance for the gas phase is given by the Navier-Stokes equation, modified to include an interphase momentum transfer term :

$$\frac{\partial}{\partial t}(\epsilon_g \rho_g \mathbf{v}_g) + \nabla \cdot (\epsilon_g \rho_g \mathbf{v}_g \mathbf{v}_g) = \nabla \cdot \bar{\bar{\tau}}_g + \epsilon_g \rho_g \mathbf{g} + -\epsilon_g \nabla P - \beta(\mathbf{v}_g - \mathbf{v}_s) \qquad (3)$$

where $\bar{\bar{\tau}}$ is the viscous stress tensor, $\mathbf{g}$ is the gravity acceleration, P is the thermodynamic pressure, and β is the interphase momentum transfer coefficient. The solids phase momentum balance is given by :

$$\frac{\partial}{\partial t}(\epsilon_s \rho_s \mathbf{v}_s) + \nabla \cdot (\epsilon_s \rho_s \mathbf{v}_s \mathbf{v}_s) = \nabla \cdot \bar{\bar{\tau}}_s + \epsilon_s \rho_s \mathbf{g} + -\epsilon_s \nabla P - \nabla P_s^* + \beta(\mathbf{v}_g - \mathbf{v}_s) \qquad (4)$$

where P_s^* is the solids pressure obtained from the kinetic theory of granular flow, as discussed below. Both the shear viscosity and the bulk viscosity are used in the viscous stress tensor, which is discussed by Bird et al. (1960).

Kinetic theory of granular flow

Equivalent to the thermodynamic temperature for gases, the granular temperature can be introduced as a measure for the energy of the fluctuating velocity of the particles. The granular temperature is defined as

$$\Theta_s = \frac{1}{3}\mathbf{v}'^2 \qquad (5)$$

where Θ_s is the granular temperature, and $\mathbf{v}'$ is the solids fluctuating velocity. The equation of conservation of the solids fluctuating energy can be found in Ding and Gidaspow (1990) :

$$\frac{3}{2}\left[\frac{\partial}{\partial t}(\epsilon_s \rho_s \Theta_s) + \nabla \cdot (\epsilon_s \rho_s \Theta_s)\mathbf{v}_s\right] = \left(-\nabla P_s^* \bar{\bar{I}} + \bar{\bar{\tau}}_s\right) : \nabla \mathbf{v} + \nabla \cdot (k_\Theta \nabla \Theta_s) - \gamma_\Theta + \Phi_\Theta \qquad (6)$$

where k_Θ is the diffusion coefficient, γ_Θ is the dissipation of fluctuating energy, and Φ_Θ is the exchange of fluctuating energy between the phases.

The dissipation of fluctuating energy is described by Jenkins and Savage (1983) :

$$\gamma_\Theta = 3(1 - e^2)\epsilon_s^2 \rho_s g_0 \Theta_s \left(\frac{4}{d_s}\sqrt{\frac{\Theta_s}{\pi}} - \nabla \cdot \mathbf{v}_s\right) \qquad (7)$$

where g_0 is the radial distribution function, which is discussed below, e is the coefficient of restitution of colliding particles, and d_s is the particle diameter.

The solids pressure represents the solids phase normal forces due to particle-particle interactions. Its description based on the kinetic theory of granular flow was developed by Jenkins and Savage (1983) and Lun et al. (1984). In this approach both the kinetic and the collisional influences are taken into account. The kinetic part describes the influence of particle translations, whereas the collisional term accounts for the momentum transfer by direct collisions. The solids pressure of Lun et al. (1984) is used in this work :

$$P_s^* = \epsilon_s \rho_s \Theta_s (1 + 2 g_0 \epsilon_s (1 + e)) \qquad (8)$$

The bulk viscosity is a measure for the resistance of a fluid against compression. It is obvious that the importance of the bulk viscosity depends strongly on the velocity gradients. In a fluidised bed, the bulk viscosity and the shear viscosity are in the same order of magnitude,

and thus the bulk viscosity should not be neglected, as is done in simulating Newtonian fluids. The equation of Lun et al. (1984) is used in this work :

$$\lambda_s = \frac{4}{3}\epsilon_s \rho_s d_s g_0 (1+e)\sqrt{\frac{\Theta_s}{\pi}} \tag{9}$$

where λ_s is the bulk viscosity of the solids phase.
Whereas pressure and bulk viscosity describe normal forces, the shear viscosity accounts for the tangential forces. It was shown by Lun et al. (1984) that it is possible to combine different inter-particle forces and to use a momentum balance similar to that of a true continuous fluid. Similar to the solids pressure, a solids phase viscosity can be derived from the kinetic theory. The shear viscosity is built up out of two terms : one term for the dilute region and one term for the dense region. In literature different expressions for the solids shear viscosity can be found. In this work the approach of Gidaspow et al. (1982) is used, because this approach is validated by comparison with measured data :

$$\mu_s = \frac{4}{5}\epsilon_s \rho_s d_s g_0 (1+e)\sqrt{\frac{\Theta_s}{\pi}} + \ldots$$
$$\ldots + \frac{2\frac{5\sqrt{\pi}}{96}\rho_s d_s \sqrt{\Theta_s}}{(1+e)\epsilon_s g_0}\cdot\left[1+\frac{4}{5}g_0\epsilon_s(1+e)\right]^2 \tag{10}$$

where μ_s is the shear viscosity of the solids phase.
In the extreme dense regions of the bed ($\epsilon_s \approx \epsilon_{s,max}$), the particle stresses are dominated by inter-particle friction rather than by collisions and fluctuating motion. The two-dimensional stress tensor for a granular material which is about to yield is proposed by Sokolovski (1965) and Jackson (1983) :

$$\mu_s = \frac{P_s^* \cdot \sin\phi}{\epsilon_s\sqrt{\frac{1}{6}\left(\left(\frac{\partial u_s}{\partial x}-\frac{\partial v_s}{\partial y}\right)^2+\left(\frac{\partial v_s}{\partial y}\right)^2+\left(\frac{\partial u_s}{\partial x}\right)^2\right)}\ldots}$$
$$\ldots\frac{}{\sqrt{+\frac{1}{4}\left(\frac{\partial u_s}{\partial y}+\frac{\partial v_s}{\partial x}\right)^2}} \tag{11}$$

where ϕ is the angle of internal friction, u and v are the velocity components, and x and y are the Cartesian directions of u and v.
The radial distribution function used in the equations above is the equilibrium radial distribution at particle contact derived from statistical mechanics. It can be seen as a measure for the probability of inter-particle contact. The equation of Ding and Gidaspow (1990) is used in this work :

$$g_0 = \frac{3}{5}\left[1-\left(\frac{\epsilon_s}{\epsilon_{s,max}}\right)^{\frac{1}{3}}\right]^{-1} \tag{12}$$

where $\epsilon_{s,max}$ is the maximum solids packing, usually between 0.6 and 0.7.
Instead of solving the complete balance of the solids fluctuating energy, equation (6), an algebraic expression was proposed by Syamlal et al. (1993) . This approach assumes that the granular energy is dissipated locally, neglecting the convection and diffusion, and retaining only the generation and the dissipation terms, resulting to :

$$0 = \left(-P_s^*\overline{\overline{I}} + \overline{\overline{\tau}}_s\right) : \nabla \mathbf{v}_s - \gamma_\Theta \tag{13}$$

This approach is only valid under the assumption that the volume fraction of the solids phase stays high, and the velocity of the solids phase stays relatively low. In this regime most granular energy is dissipated locally, and little is left to flow away. Equation (13) can then be rewritten into :

$$\Theta_s = \left(\frac{-(K_1\epsilon_s+\rho_s)\,tr\left(\overline{\overline{D}}_s\right)+\ldots}{\ldots+\sqrt{(K_1\epsilon_s+\rho_s)^2\,tr^2\left(\overline{\overline{D}}_s\right)+4K_4\epsilon_s\cdot}\ldots}{\ldots\frac{\ldots}{\ldots\frac{\left[2K_3\,tr\left(\overline{\overline{D}}_s^2\right)+K_2\,tr^2\left(\overline{\overline{D}}_s\right)\right]}{2\epsilon_s K_4}}}\right)^2 \tag{14}$$

where $\overline{\overline{D}}_s$ is the solids strain rate tensor, and with the abbreviations :

$$K_1 = 2(1+e)\rho_s g_0$$
$$K_2 = \frac{4}{3\sqrt{\pi}}d_s\rho_s(1+e)\epsilon_s g_0 - \frac{2}{3}K_3$$
$$K_3 = \frac{d_s\rho_s}{2}\left(\frac{\sqrt{\pi}}{3(3-e)}\ldots\right.$$
$$\left.\ldots\left[1+\frac{2}{5}(1+e)(3e-1)\epsilon_s g_0\right]+\frac{8\epsilon_s}{5\sqrt{\pi}}g_0(1+e)\right)$$
$$K_4 = \frac{12(1-e^2)\rho_s g_0}{d_s\sqrt{\pi}}$$

When using this algebraic equation in stead of solving the balance for the granular temperature, much faster convergence is obtained during simulations. It has been shown by Boemer et al. (1995) that using this approach hardly affects the granular temperature in the bubbling regime.

Interphase momentum exchange

In this work the interphase drag function of Syamlal et al. (1993) is used. This drag function is based upon Richardson and Zaki (1954), Dalla Valle (1948), and Garside and Al-Dibouni(1977) :

$$\beta = \frac{3}{4}C_D\frac{\epsilon_s\epsilon_g\rho_g}{V_r^2 d_s}\cdot|\mathbf{v}_g-\mathbf{v}_s| \tag{15}$$

with

$$C_D = \left(0.63+4.8\sqrt{\frac{V_r}{Re}}\right)^2$$
$$V_r = 0.5\cdot$$
$$\left(a-0.06Re+\sqrt{(0.06Re)^2+0.12Re(2b-a)+a^2}\right)$$
$$a = \epsilon_g^{4.14}$$
$$b = \begin{cases} 0.8\epsilon_g^{1.28} & \text{if } \epsilon_s \geq 0.15 \\ \epsilon_g^{2.65} & \text{if } \epsilon_s < 0.15 \end{cases}$$
$$Re = \frac{d_s\rho_g\cdot|\mathbf{v}_g-\mathbf{v}_s|}{\mu_g}$$

where C_D is the drag coefficient, V_r is the ratio of terminal velocity of a group of particles to that of an isolated

particle, Re is the particle Reynolds number, and μ_g is the gas viscosity.
This approach is only valid if the distribution of particles on the size of the grid cells can be assumed homogeneous. The size of the grid cells in multiphase simulations is in the order of one square centimetre. Especially in systems with very low solids concentration, like for instance circulating fluidised beds, the number of particles in a grid cell is largely fluctuating compared to the total number of particles, and this approach can give incorrect results.

Simulations

Simulation code

The differential equations (1), (3) and (4) mentioned in the previous section all express a conservation principle and are solved on a unit-volume basis. Thus the conservations need to yield over all possible finite volumes covering the whole problem space. Solving differential equations this way is called finite volumes. The differential equations express the conservation over an infinitesimal control volume and need to be discretised over the used finite volumes. This mathematical process is described by Patankar (1980).
The simulations were carried out with the commercial CFD code CFX4.1c from AEA Technology, Harwell, UK. This package allows free implementation of extra equations, boundary conditions, and differencing schemes. The granular kinetic theory and the granular equations described in the previous section were implemented into this code. The discretisation used by CFX is the so called Rhie-Chow (1983) algorithm. This algorithm can be used with a non staggered grid : all the discretised variables are stored at the same boundary points. For solving the difference equations obtained from the differential equations, the higher order TVD scheme minmod is used. This TVD scheme incorporates a modification to the higher-order upwind scheme. Sokolichin et al. (1997) have shown that solutions obtained with the TVD scheme result in less numerical diffusion than lower order schemes. Less numerical diffusion leads to a sharper interface between the gas and the solid boundary (e.g. at bubbles or at the freeboard). The solution of the pressure from the momentum equations requires a pressure correction equation, correcting the pressure and the velocities after each iteration of the discretised momentum equations. In this work the SIMPLE algorithm developed by Patankar (1980) is used for this purpose. The calculated pressure is used to calculate the density of the gas phase.

Fluidisation conditions

The values used for the parameters needed in the simulations can be seen in Table 1. The simulated fluidised bed is a two-dimensional square column. Air at ambient temperature and pressure is used for the fluidising gas. The gas is treated compressible and thus the density is coupled to the pressure, according to the ideal gas law. For the solids, uniform sized glass beads were used. It has been shown by De Groot (1967) that the diameter distribution has a large influence on the fluidisation behaviour of the granular material. De Groot states it is difficult to fluidise monodisperse solids, especially in larger beds. There is however little known yet about the exact cause and effect and it is unknown how a physical diameter distribution should be implemented into a TFM, and what the effect would be. The TFM is not an exact model of a fluidised granular material, and it is questionable whether an implemented diameter distribution or not would make a large difference.
The size of the time step influences two effects : the convergence of the iterations regarding the solution of the differential equations, and the computation time. The time step used for the highest simulated fluidisation velocity, (i.e., four times U_{mf}) is $1.0 \cdot 10^{-4} s$ and for the lowest velocity (i.e., two times U_{mf}) twice this size is used. Both were checked to be sufficiently small.
The size of the grid spacing in multiphase flow is of the order of one square centimetre. This is found to be an optimum between computational effort and numerical diffusion. The larger the grid spacing is, the more numerical diffusion will take place. At high fluidisation velocities, diffusion of mass is less important than at lower fluidisation velocities. In this work it is found that lower fluidisation velocities require a finer mesh. Using a coarse mesh at lower fluidisation velocities leads to lower porosities in bubbles, and thus to less realistic results. The mesh chosen in this work for two times U_{mf} is $\Delta x = 7.0 \cdot 10^{-3} m$, and for four times U_{mf} is $\Delta x = 1.0 \cdot 10^{-2} m$. These values lead to similar volume fraction inside bubbles at all simulated fluidisation conditions.

Boundary and initial conditions

All simulations are carried out in a pseudo two-dimensional square space in which there are no front and back wall effects. In the simulations particles cannot travel freely in the third dimension : the momentum equations are only solved for two dimensions. Numerically this can be seen as two symmetry planes placed right in the front and at the back of the fluidised bed.
The left and right wall of the fluidised bed are treated as no slip boundary conditions for the gas phase : the velocity of the gas phase is set to zero at the wall. For the solids phase a different condition should be used : particles can move downwards while touching the wall. It seems not very important what kind of slip condition is chosen at the wall, as long as particles are able to fall down at the wall. In this work a free slip condition is chosen : the particles find no hinder in their downward or upward velocity when they are near a wall.
The boundary condition at the top of the fluidised bed is a so-called pressure boundary. The pressure in the mesh cells at the top of the fluidised bed are fixed at a specific value. Neumann boundary conditions are applied to the gas flow velocity. This is also called 'fully developed flow' : the derivatives of the upward velocity in the horizontal direction are assumed zero. It is important that the freeboard of the fluidised bed is high enough, so that fully developed flow can be physically expected.
From the momentum balances, the mass flux, containing the concentration, is solved. If the concentration is zero or within the computational inaccuracy, this can lead to unrealistic values for the particle velocity field, resulting in an unrealistic drag force and that leading to an unrealistic gas velocity field. For that reason, a very small solids concentration ($\sim 10^{-6}$) for the particle phase is

Table 1. List of values of model parameters used in the simulations.

Symbol	Description	Value	Comment or reference
ρ_s	solids density	$2600\,kg\,m^{-3}$	glass beads
ρ_g	gas density	$1.28\,kg\,m^{-3}$	air at ambient conditions
d_p	particle diameter	$500\,\mu m$ (Geldart B type)	no size distribution
e	coefficient of restitution	0.60	Boemer et al. (1995)
ϵ_{max}	maximum solids packing	0.61	Syamlal et al. (1993)
ϕ	angle of internal friction	25°	Johnson and Jackson (1987)
U_{mf}	minimum fluidisation velocity	$0.25\,ms^{-1}$	from Ergun (1952)
Δt	time step	$1.0\,10^{-5}\,s < \Delta t < 2.0\,10^{-4}\,s$	for convergence
Δx	mesh spacing	$6.0\,10^{-3}\,m < \Delta x < 1.0\,10^{-2}\,m$	to reduce numeric diffusion
Θ_s	granular temperature	$10^{-5} m^2 s^{-2} < \Theta_s < 0.1\,m^2 s^{-2}$	Balzer and Simonin (1993)
U_0	superficial gas velocity	$0.5\,ms^{-1} < U_0 < 1.0\,ms^{-1}$	a range is used
D_t	column diameter	$0.2\,m < D_t < 0.4\,m$	a range is used
H_t	column height	$0.6\,m$	fixed value
H_{mf}	settled bed height	$0.34\,m$	fixed value

set in the top cells, leading to particle 'leakage' into the fluidised bed (Balzer and Simonin, 1996). This way the whole freeboard is filled with a very small number of particles. The number of particles in the freeboard is chosen small enough not to have any influence on the physics in the fluidised bed.

At the bottom of the fluidised bed, the gas inflow is specified. This is called a Dirichlet boundary condition. In the beginning of the simulation a small perturbation is specified in one of the cells of the bottom. This is to break the horizontal symmetry. In an actual fluidised bed this is caused by the random packing of the particles. The distributor is made impenetrable for the solids phase : the solids downward velocity is set to zero in the bottom cells.

For the initial condition the bottom half of the bed is filled with particles at a particle concentration of 0.58. The gas flow in the bed is set to minimum fluidisation velocity at $t = 0$. In the freeboard a very small number of particles is set, as was explained above.

Classical bubble size and velocity relations

A lot of experimental work has been done in the 70's and 80's regarding the bubble behaviour in gas-solid fluidised beds. The Darton et al. (1977) bubble model is a generally accepted semi-empirical model for bubble growth. The model is based upon the preferred paths of bubbles where the distance travelled by two neighbouring bubbles before coalescence is proportional to their lateral separation. The proposed equation is :

$$D_b = 0.54(U_0 - U_{mf})^{0.4}(h + 4\sqrt{A_0})^{0.8}/g^{0.2} \quad (16)$$

where D_b is the bubble diameter, h is the height of the bubble above the distributor, and A_0 is the 'catchment area' which characterises the distributor; 0.54 is the only experimentally determined constant. This model is not applicable to slug flow, nor to Geldart C powders.

Werther and Molerus (1973) developed a small capacitance probe to measure the bubble diameter and the bubble velocity. This capacitance probe can be placed in the fluidised bed, at different heights and radial positions. The bubble velocity can be determined by placing two capacitance probes above each other, and correlating the data obtained. The main problem in this approach is translating the measured pierced lengths into an average bubble diameter with a distribution. To accomplish this, Werther (1974) assumed the bubble shape to be elliptical. Knowing the total number of bubbles that have passed the probe, he determined an average bubble diameter and diameter distribution from the measured pierced lengths.

Davidson and Harrison (1963) proposed a bubble rise velocity according to the two phase theory of fluidisation :

$$u_b = U - U_{mf} + \varphi\sqrt{gd_b} \quad (17)$$

where φ is the analytically determined square root of the Froude number of a single rising bubble in an infinitely large homogeneous area. Pyle and Harrison (1967) have determined that $\varphi = 0.48$ for a two dimensional geometry, whereas in three dimensions $\varphi = 0.71$. Equation 17, however, did not satisfy the results obtained by Werther (1974). Hilligardt and Werther (1986) explained the differences between Werther's measurements and the two phase flow equation by the following observations :

1. under normal operating conditions for bubble formation without slugging, the visible flow rate is clearly lower than the excess gas velocity $(U - U_{mf})$;
2. bubbles of a given size rise faster in a fluidised bed of larger diameter.

They proposed an adapted equation for the bubble rise velocity :

$$u_b = \psi(U - U_{mf}) + \varphi\nu\sqrt{gd_b} \quad (18)$$

to correct for the two differences mentioned. Hilligardt and Werther (1986) have determined empirical correlations for the parameters ψ and ν for different types of solids. They have done experiments with similar particles as used in this work ($\rho_s = 2640 kg\,m^{-3}$, $d_p = 480\mu m$), and have used these simulations to establish the values for the parameters of Geldart group D particles, because Molerus (1982) has characterised this solid under group D. The parameter ψ describes the deviation of the visible bubble flow rate, $\dot{V}_b$, from the two phase theory :

$$\psi = \frac{\dot{V}_b}{U - U_{mf}} \quad (19)$$

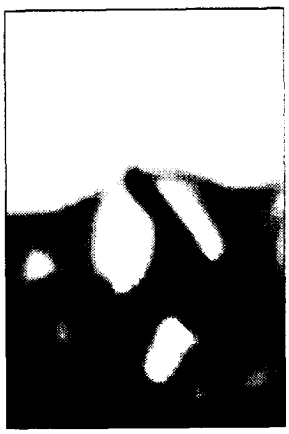

Figure 1. *The visual representation of a simulation of 0.4 m width column at 4 times U_{mf}.*

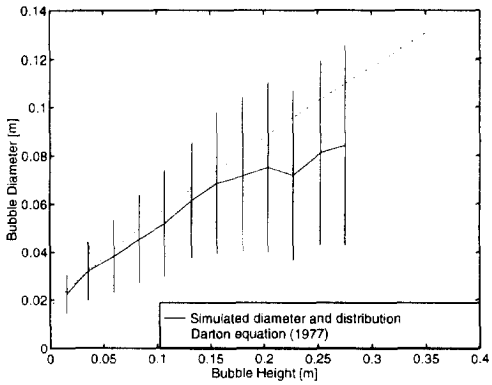

Figure 2. *Bubble diameters versus bed height at 2 times U_{mf} in a 0.4 m width column.*

Values for ψ have been experimentally obtained by Hilligardt and Werther (1986) :

$$\psi = \begin{cases} 0.26 & \frac{h}{D_t} < 0.55 \\ 0.35 \left(\frac{h}{D_t}\right)^{0.5} & 0.55 \leq \frac{h}{D_t} \leq 8 \end{cases} \quad (20)$$

for Geldart group D particles. This was later simplified by Kunii and Levenspiel (1991) to a similar, but bubble height independent formula.

The parameter ν accounts for that part of the deviation from the behaviour from a single bubble, which is not reflected by the additive term $\psi(U - U_{mf})$. Hilligardt and Werther (1986) have experimentally determined for Geldart group D solids :

$$\nu = 0.87 \quad (21)$$

CFD simulation results

The fluidised state of the bed can be visualised by plotting different grey tones, assigned to different solid volume fraction regions, in the grid cells. This is done in Figure 1 by assigning darker grey tones to increasing solid volume fractions.

In this paper a bubble is defined as an area where the solid volume fraction is below a certain value. The value in this work is chosen at 20%. This value is also used by other authors and does not depend on the mesh coarseness : the value of 20% lies before the largest solid volume fraction gradient leading to a bubble edge. To ensure this, the mesh for the lower fluidisation velocities is finer than for higher velocities. Confined areas with more than one cell with a solid volume fraction below 20% are defined as bubbles. The diameter of this bubble is calculated as if its shape is circular and the diameters and centres of all bubbles in the bed are recorded. Bubble velocities are determined by studying the bubble diameter and centre in consecutive time steps, thus enabling the calculation of the complete bubble trajectory.

The main object of this work is to validate the outcome of the CFD model with existing empirical equations for bubble size and velocity. This validation can be difficult, because it is not always exactly clear what authors have measured in reality : have they taken all the bubbles into account, or only the larger bubbles; have they included effects as coalescence, break-up, and wall effects? Experimentally it can be very hard to obtain precise physical data from a fluidised bed, whereas simulations like in this work produce an abundance of data. *When comparing a model to measurements, it is important to retrieve similar data from the model as is retrieved from the measurements.* For the empirical models of Hilligardt and Werther (1986) and Darton et al. (1977), bubbles touching the column walls were not considered. The determination of the bubble velocity by Werther (1974) was done by not taking effects like coalescence and break-up during the observation into account. These effects should not be considered when comparing the predicted bubble trajectories to the correlation of Hilligardt and Werther (1986). For comparison with the Darton et al. (1977) equation, the bubbles in each simulation are divided into twelve categories of increasing bubble diameter. Figure 2 shows the bubble diameter and the distribution of each category together with the estimated average bubble diameter by the Darton equation for one condition. It can be seen that the predicted bubble diameters are slightly smaller in the higher part in the fluidised bed, but not in disagreement. This can be due to a deficiency of the used measuring technique by Darton et al. (1977) in measuring very small bubbles.

The bubble rise velocities versus the bubble diameters are shown in Figure 3. This figure shows an enormous spread in bubble rise velocities, due to coalescence, break-up, and bubbles interacting directly with the wall. Figure 4 shows the same bubbles averaged into eight classes with increasing bubble diameter. In can be seen that especially smaller bubbles show deviating behaviour : the average small bubbles rise faster through the bed than predicted by Hilligardt and Werther (1986), whom have only used bubbles of $0.04m$ and larger to establish their correlation; a wake of a bubble has a larger effect on a trailing small bubble than on a trailing larger one. Figure 5 shows part of bubble trajectories without coalescence, break-up, and bubbles touching the wall. The symbol '+' is used for bubbles which are not within $\pm$ 30% of the Darton et al. (1977) equation, and the symbol 'x' is used for the remaining bubbles. In this figure also the equation proposed by Hilligardt and Werther (1986) is shown. The unaffected bubble trajectories averaged in classes and a

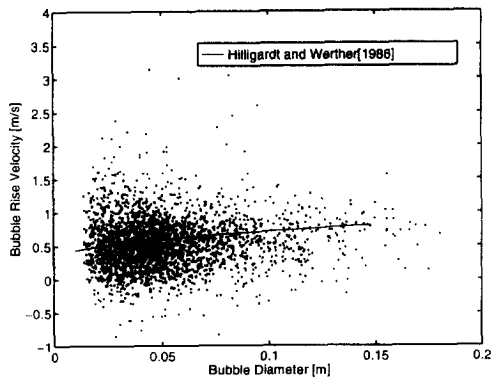

Figure 3. *Bubble rise velocity versus bubble diameter at 4 times U_{mf} in a 0.4 m width column. All bubbles predicted from the simulation are shown.*

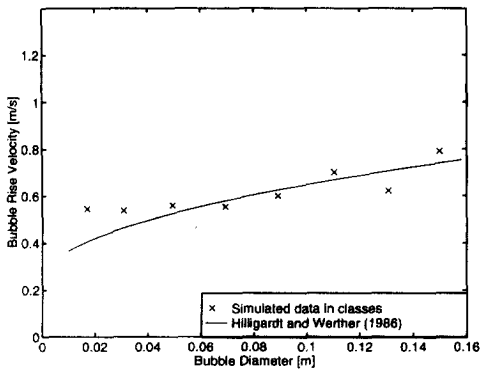

Figure 4. *Bubble rise velocity versus bubble diameter at 4 times U_{mf} in a 0.4 m width column : the bubbles of Figure 3 have been averaged into eight classes.*

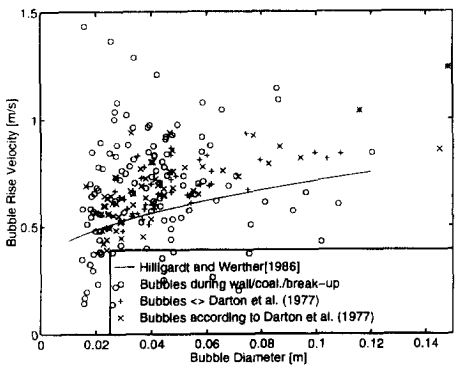

Figure 5. *Bubble rise velocity versus bubble diameter at 4 times U_{mf} in a 0.4 m width column. Bubbles affected by coalescence, break-up, and bubbles touching the wall during the calculation of their velocity are shown with 'o', while other bubbles with 'x' or '+'.*

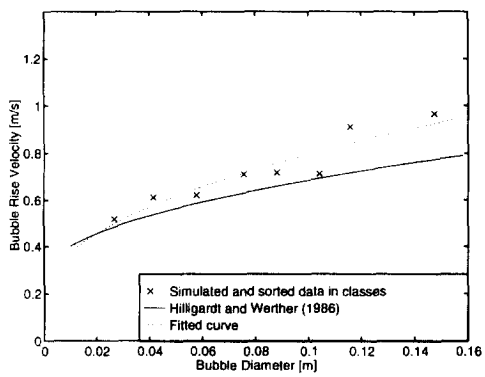

Figure 6. *Bubble rise velocity versus bubble diameter at 4 times U_{mf} in a 0.4 m width column. Predicted bubbles not affected by coalescence, break-up, and bubbles touching a wall during the calculation of the velocity grouped into eight classes.*

fit of this data is shown in Figure 6. The values for the coefficients ψ and ν proposed by Hilligardt and Werther (1986), and the resulting values of the fits from all simulated fluidisation conditions are shown in Table 2. For the determination of the parameters at each fluidisation condition, over 3000 bubbles are used. The simulation results are in reasonable agreement with the values proposed by Hilligardt and Werther (1986). One of the main issues in testing the CFD model is comparing the abundance of data out of each simulation to the empirical relations developed by measurements. Measuring techniques and the processing of the outcome of these measurements do not always reflect the exact physical behaviour of a system. In the Hilligardt and Werther (1986) bubble model, coalescence, break-up, and direct wall effects are not included. This work shows however, that these effects are very important in the bubble behaviour, especially with smaller bubbles. Figure 3 shows that a large number of bubbles do coalesce, break-up, or have wall interactions, and that these bubbles do not necessarily have the rising velocity predicted by the Hilligardt and Werther (1986) equation.

Conclusions

The predicted values of the bubble diameter at a certain bed height are in agreement with the Darton et al. (1977) bubble equation.

The comparison of the parameters ψ and ν with Hilligardt and Werther (1986) show that the values are in the same order of magnitude, and that the model of Hilligardt and Werther (1986) is in agreement with the (larger) bubbles predicted by simulations. In this work, however, some dependency is seen of both parameters upon the fluidisation condition. Hilligardt and Werther do not state which fluidisation conditions they have used to obtain the values for ψ. Possibly ψ is less fluidisation condition independent as reported by Hilligardt and Werther (1986).

The large abundance of data obtained from a simulation gives much information about the dynamic behaviour in fluidised beds and can be a very valuable tool, not only in the validation of existing empirical correlations, but also in the improvement of existing correlations, the determination of new correlations, or the calculation of specific physical properties of a certain configuration.

Table 2. *Comparison of calculated values for ψ and ν from the CFD model simulations at different column diameters and fluidisation velocities with the values from the Hilligardt and Werther (1986) model.*

		This work	H. & W.	This work	H. & W.	This work	H. & W.
		Column diameter					
U_0 [m/s]	Parameter [-]	20 cm		30 cm		40 cm	
0.50	ψ	1.1	0.26 - 0.35	1.0	0.26 - 0.35	0.90	0.26 - 0.35
	ν	0.62	0.87	0.61	0.87	0.63	0.87
0.625	ψ	0.71	0.26 - 0.35	0.62	0.26 - 0.35	0.81	0.26 - 0.35
	ν	0.74	0.87	0.70	0.87	0.66	0.87
0.75	ψ	0.32	0.26 - 0.35	0.40	0.26 - 0.35	0.48	0.26 - 0.35
	ν	0.79	0.87	0.87	0.87	0.95	0.87
0.875	ψ	0.24	0.26 - 0.35	0.24	0.26 - 0.35	0.49	0.26 - 0.35
	ν	1.01	0.87	1.26	0.87	0.81	0.87
1.0	ψ	0.22	0.26 - 0.35	0.34	0.26 - 0.35	0.50	0.26 - 0.35
	ν	0.86	0.87	0.91	0.87	0.74	0.87

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