A comparison of first and second order spatial scheme for simulation of a bubbling fluidised bed

B. Halvorsen & V. Mathiesen
Telemark University College, Norway
Telemark Technological R&D Centre (Tel-Tek), Norway

Abstract

This paper presents an experimental and computational study of the bubble formation in a bubbling fluidised bed. The simulations are performed using a computational fluid dynamics (CFD) model named FLOTARCS-MP-3D proposed by Mathiesen et al. [1]. In order to reduce numerical diffusion and to study the effect of numerical schemes, the spatial first order upwind scheme is extended to second order in the momentum equations. Second order scheme may give unphysical and unbounded solutions. To avoid this, different flux limiters are tested. A two-dimensional lab-scale bubbling fluidised bed with a central jet is build. The bubble formation in the bed is visualised using a digital video camera. A comparison of simulation results with first and second order schemes shows that the numerical diffusion is reduced significantly, and that a more physically shaped bubble is formed with second order scheme.

1 Introduction

Computational fluid dynamics (CFD) of multiphase flow processes provides a new tool for design and optimisation of multiphase flow systems such as fluidised reactors. However, in order to be able to calculate complex industrial fluidised bed reactors, the bubble formation has to be calculated correctly. Both Symalal [2] and Halvorsen and Mathiesen [3] demonstrated that simulations performed with first order convective upwind scheme in the model give bubbles with an unphysical pointed shape, and concluded that this is probably due to numerical diffusion. This paper discusses the changes in bubble shape when first order upwind scheme (FOU) is replaced by second order upwind scheme (SOU).
2 Mathematical model

The simulation is performed using a CFD model (FLOTRACS-MP-3D) proposed and described in detail by Mathiesen et al [1]. The model is based on a multi-fluid Eulerian description of the phase. The kinetic theory for granular flow forms the basis for the turbulence modelling of the solid phases. The gas phase turbulence is modelled by a sub-grid scale (SGS) model, Deardorff [4]. The largest scales are simulated directly, whereas the small scales are modelled by the SGS turbulence model. The numerical solution procedure is modified in this study by including second order convective upwind scheme for the momentum equations.

2.1 Governing equations

2.1.1 Continuity equations
The continuity equation for phase \( m \) (gas or solid) is given by:

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m) + \frac{\partial}{\partial x_i} (\varepsilon_m \rho_m U_{i,m}) = 0
\]  

where \( \varepsilon, \rho \) and \( U_i \) are the phase volume fraction, density, and \( i \)-th direction velocity component for phase \( m \), respectively. No mass transfer is allowed between the phases.

2.1.2 Momentum equations
The momentum equation in the \( j \)-direction for phase \( m \) may be expressed as:

\[
\frac{\partial}{\partial t} (\varepsilon_m \rho_m U_{j,m}) + \frac{\partial}{\partial x_j} (\varepsilon_m \rho_m U_{i,m} U_{j,m}) = -\varepsilon_m \frac{\partial p}{\partial x_j} + \frac{\partial \Pi_{i,j,m}}{\partial x_i} + \varepsilon_m \rho_m g_j + \Phi_{mk} (U_{j,k} - U_{j,m})
\]

\( p \) is fluid pressure, \( g_j \) is \( j \)-direction component of gravity and \( \Phi_{mk} \) is the drag coefficient between the \( m \) and \( k \) phases. The terms on the right side represent pressure forces, viscous forces, mass forces and drag forces respectively.

2.1.3 Granular temperature equations
In recent continuum models, e.g. Mathiesen et al. [1], Ding and Gidaspow [5] and Goldschmidt et al. [6], equations according to kinetic theory of granular flow are incorporated. This theory describes the dependence of the rheologic properties of the fluidised particles on local particle concentration and the random fluctuating motion of particles due to particle-particle collisions.
The transport equation for granular temperature, \( \theta \), is given by:

\[
\frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \varepsilon_s \theta_s \theta_s \right) + \frac{\partial}{\partial x_i} \left( \varepsilon_s \theta_s U_{i,s} \theta_s \right) \right] = \left( \Pi_{i,s} : \frac{\partial U_{j,s}}{\partial x_i} \right) \\
+ \frac{\partial}{\partial x_i} \left( \kappa_s \frac{\partial \theta_s}{\partial x_i} \right) - \gamma_s - 3 \Phi_{s} \theta_s
\]  

(3)

The terms on the right side represent granular temperature production, conductivity of granular temperature, dissipation due to particle-particle collisions and dissipation due to fluid-particle interaction.

2.2 Numerical solution procedure

The governing equations are solved by a finite volume method where the calculation domain is divided into a finite number of non-overlapping control volumes. Volume fraction, density and granular temperature are stored at main grid points placed in centre of the control volumes. Staggered grid arrangements are used for the velocity components that are stored at the main control volume surfaces. Figure 1 shows a scalar control volume for a two-dimensional Cartesian situation and in Figure 2 a velocity control volume is shown.

The conservation equations are integrated in space and time. The integration is performed using first or second order upwind differencing in space and fully implicit in time.

Due to strong coupling between the phases through the drag forces, the two-phase partial elimination algorithm (PEA) is used to decouple the drag forces. The interphase-slip algorithm (IPSA) is used to take care of the coupling between the continuity and the velocity equations.
2.2.1 First order upwind scheme (FOU)

From the general differential equation:

\[
\frac{\partial}{\partial t} (\rho \Phi) + \frac{\partial}{\partial x_i} (\rho U_i \Phi) = \frac{\partial}{\partial x_i} \left( \frac{\partial \Phi}{\partial x_i} \right) + S_{\Phi,i}
\]

a general discretisation equation for the dependent variable \( \Phi \) for a one-dimensional system is obtained.

\[
ap_r \Phi_P = a_E \Phi_E + a_W \Phi_W + b
\]

Where \( b \) is the constant part of the source term. The value of \( \Phi \) in point \( P \) becomes a linear combination of \( \Phi \) in the neighbour points \( W \) and \( E \). The coefficients in the neighbour points depend on how \( \Phi \) varies between the main grid nodes, and include convection and diffusion. For the FOU difference scheme the coefficients of the neighbouring points can be written as, Patankar [7]:

\[
a_W = \max(F_w,0) + D_W \quad a_E = \max(-F_e,0) + D_E
\]

The variables, \( F \) and \( D \), represent the convective and the diffusive fluxes at cell faces and are defined according to:

\[
F_e = (\rho U)_e \Delta y \quad F_w = (\rho U)_w \Delta y \quad D_e = \frac{\Gamma_e \Delta y}{\delta x_e} \quad D_w = \frac{\Gamma_w \Delta y}{\delta x_w}
\]

The general transport coefficient at the east control volume surface is expressed as:

\[
\Gamma_{\Phi,e} = \frac{2 \rho \Gamma_e \delta x_e}{\Gamma_p \Delta x_E + \Gamma_e \Delta x_P}
\]

2.2.1 Second order upwind scheme (SOU)

The principle of the SOU scheme is illustrated in Figure 3. The cell face value of \( \Phi \) is estimated from the two upstream neighbouring nodes by linear extrapolation.

![Figure 3: The principle of second order upwind scheme.](image-url)
The value of $\Phi_e$ can be expressed by:

$$\Phi_e = \Phi_p + (\Phi_p - \Phi_w) \left( \frac{\partial x}{\partial x} \right)_{wp} \text{ if } F_e > 0$$

$$\Phi_e = \Phi_E + (\Phi_E - \Phi_{EE}) \left( \frac{\partial x}{\partial x} \right)_{EE} \text{ if } F_e < 0$$

$$a_p \Phi_p = a_E \Phi_E + a_w \Phi_w + a_{EE} \Phi_{EE} + a_{ww} \Phi_{ww} + b$$

For uniform grid size the coefficients of the neighbouring points become:

$$a_E = D_e + \frac{3}{2} \max(-F_e,0) + \frac{1}{2} \max(-F_w,0)$$

$$a_w = D_w + \frac{3}{2} \max(F_w,0) + \frac{1}{2} \max(F_e,0)$$

$$a_{EE} = -\frac{1}{2} \max(-F_e,0)$$

$$a_{ww} = -\frac{1}{2} \max(F_w,0)$$

The SOU scheme is unbounded and may generate oscillations around sharp gradients, Hirsch [8]. Introduction of non-linear flux limiters into the scheme solves this problem. Such limiters are derived on the basis of the total variation diminishing (TVD) conditions, which ensure that no new local extrema are created and that the value of an existing local minimum/maximum must be non-decreasing/non-increasing. The SOU-scheme for $\Phi_e$ with TVD limiters can be written as:

$$\Phi_e = \Phi_p + \frac{1}{2} \Psi_e (r_e)(\Phi_p - \Phi_w) \text{ if } F_e > 0$$

where $\Psi_e(r_e)$ is the flux limiter and $r_e$ is the limiter argument.

$$r_e = \frac{\Phi_E - \Phi_p}{\Phi_p - \Phi_w}$$

Several different flux limiters are proposed to ensure the TVD conditions. In this work the following flux limiters are tested:

Van Leer limiter: $\Psi_e (r_e) = \frac{r_e + |r_e|}{(1 + r_e)}$ (14)

Superbee limiter: $\Psi_e (r_e) = \max(0, \min(2r,1), \min(r,2))$ (15)

Minmod limiter: $\Psi_e (r_e) = \max(0, \min(r,1))$ (16)

Second order accuracy is ensured by the condition $\Psi(1)=1$, and $\Psi=0$ reduces the scheme to first order accuracy.
3 Experimental and computational results

3.1 Experimental results

Bubble formation in a two dimensional bed with a central jet is studied experimentally. The experimental set-up is shown in Figure 4, and the experimental conditions are given in Table 1. PMMA (poly methyl meta acrylat) particles with volume averaged diameter and standard deviation of 128 and 25μm are applied in the experiments. The initial bed height of the fluidised bed is 25 cm. The bed is fluidised by introducing compressed air through the air distributor. Jet air is injected at a velocity of 1.5 m/s. A digital video camera is applied to measure bubble formation and velocity.

Figure 4: The experimental set-up

Table 1: Experimental conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height experimental set-up</td>
<td>63.0 cm</td>
</tr>
<tr>
<td>Width experimental set-up</td>
<td>19.5 cm</td>
</tr>
<tr>
<td>Jet area</td>
<td>0.5x2.5 cm²</td>
</tr>
<tr>
<td>Depth experimental set-up</td>
<td>2.50 cm</td>
</tr>
<tr>
<td>Mean particle size</td>
<td>128 μm</td>
</tr>
<tr>
<td>Initial bed height</td>
<td>25.0 cm</td>
</tr>
<tr>
<td>Jet velocity</td>
<td>1.5 m/s</td>
</tr>
<tr>
<td>Fluidisation velocity</td>
<td>0.02 m/s</td>
</tr>
<tr>
<td>Solid density</td>
<td>1100 kg/m³</td>
</tr>
<tr>
<td>Bulk density</td>
<td>500 kg/m³</td>
</tr>
</tbody>
</table>

Photographs from the experiments are shown in Figure 5. A bubble is created about 10 cm above the gas inlet. During the rise, the shape of the bubble changes. After 0.900 s the bubble has erupted.
3.2 Computational results

Computational set-up is given in Table 2. Simulations have been run with FOU, SOU, and with SOU with the flux limiters Van Leer, Superbee and Minmod.

<table>
<thead>
<tr>
<th>Table 2</th>
<th>Computational set-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>63.0 cm</td>
</tr>
<tr>
<td>Width</td>
<td>19.5 cm</td>
</tr>
<tr>
<td>Freeboard pressure</td>
<td>101325.0 Pa</td>
</tr>
<tr>
<td>Max. volume fraction of solids</td>
<td>0.60</td>
</tr>
<tr>
<td>Initial bed height</td>
<td>25.0 cm</td>
</tr>
<tr>
<td>Particle mean diameter</td>
<td>128 μm</td>
</tr>
<tr>
<td>Gas phase shear viscosity</td>
<td>$1.8 \times 10^{-5}$ Pa s</td>
</tr>
<tr>
<td>Horizontal grid size</td>
<td>5.0 mm</td>
</tr>
<tr>
<td>Initial void fraction</td>
<td>0.55</td>
</tr>
<tr>
<td>Vertical grid size</td>
<td>10.0 mm</td>
</tr>
<tr>
<td>Jet velocity</td>
<td>1.5 m/s</td>
</tr>
<tr>
<td>Solid density</td>
<td>1100 kg/m³</td>
</tr>
<tr>
<td>Fluidisation velocity</td>
<td>0.02 m/s</td>
</tr>
<tr>
<td>Coefficient of restitution</td>
<td>0.95</td>
</tr>
</tbody>
</table>

The simulation results with different schemes are shown in Figure 6, 7, 8, 9 and 10. Halvorsen and Mathiesen [3] showed that drag model, coefficient of restitution and number of particle phases have an effect on the bubble formation. In this work, spherical PMMA particles with a narrow particle size distribution are used, and the simulation are therefore performed with only one particle phase. Gibilaro drag model [9] is used in the simulations.
Figure 6 shows that the bubble shape is elliptical, and that FOU scheme gives an unphysical pointed bubble. This is assumed to be due to numerical diffusion. The bubble erupted after about 0.600 s.

![Figure 6: Volume fraction of solids, FOU scheme.](image)

In figure 7, 8, 9, 10 the results from the simulations with second order scheme are shown. Figure 7 confirms that the shape of the bubble becomes rounded and more spherical when SOU scheme with Superbee flux limiter is used. Another effect of using second order scheme is that the bubble velocity decreases. Figure 8 shows that simulation with SOU scheme with Van Leer flux limiter also gives a rounded bubble. A comparison of these two flux limiters shows that the bubble shape differs insignificantly, and that Superbee limiter gives the lowest bubble velocity. The simulation with Minmod flux limiter is presented in Figure 9. This simulation gives almost the same result as the simulation with Van Leer flux limiter.

![Figure 7: Volume fraction of solids, SOU with Superbee flux limiter.](image)
Simulation with second order scheme without a flux limiter is shown in Figure 10. This simulation gives the lowest bubble velocity and the most realistic bubble shape. The bubble erupts after 0.800 seconds. SOU without flux limiter gives second order accuracy, whereas the limiters can give a locally reduced accuracy. However, SOU without a flux limiter can generate oscillations around sharp gradients, and may give unphysical solutions after some time.
4. Concluding remarks

Second order upwind discretization scheme and the flux limiters Superbee, Van Leer and Minmod, are included in the CFD model FLOTRACS-MP-3D. Simulations of a two-dimensional fluidised bed were performed with first and second order discretization schemes. The simulations with FOU gave unphysical pointed, elliptical bubbles as a result of numerical diffusion. Implementation of second order scheme reduced the numerical diffusion significantly, and the simulations gave physically more realistic rounded bubbles. Second order schemes also gave a lower bubble velocity. A comparison of the results from experiments and simulations showed that SOU without flux limiter give the most realistic bubble shape and bubble velocity, but SOU without a flux limiter can generate oscillations around sharp gradients, and may give unphysical solutions after some time. The comparison of the different flux limiter showed that all the flux limiters gave a rounded bubble and that simulations with Superbee gave the lowest bubble velocity.

References