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An Explicit Method for the Packing Limit Management in Dense Gas-Solid Flow CFD Simulations on Both Structured and Unstructured Grids

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Abstract

An explicit method for limiting the volume fraction of the dispersed phase in the CFD simulations of dense gas-solid flows is described and validated both on structured and unstructured computational grids. The procedure is based on the excess solids volume correction method proposed by Lettieri et al. (2003), which has been extended in this work to non-uniform grids made of cells having different shape and size. The method has been implemented in OpenFOAM and validated through the simulation of a fluidised bed in which the superficial gas velocity has been reduced to a value close to zero.

KEYWORDS: multiphase CFD simulations, packing limit
1 INTRODUCTION

In Eulerian two-fluid simulations, the phase volume fraction $\alpha_i$ can be successfully bound between zero and one using one of the approaches proposed in the literature by Carver (1982), Spalding (1985), Carver and Salcudean (1986), Weller (2002), Rusche (2002).

It is more difficult to limit the volume fraction of a dispersed granular phase to its maximum physical value, which is not automatically respected in dense gas-solid flow simulations, if no special treatment is adopted. This is more evident in the simulation of fluidised beds operating closely at minimum fluidisation conditions, but it may also be an issue in more complex flows, where dense regions might form.

Gidaspow (1994) proposed overcoming this problem through the introduction of a solids stress modulus, which leads to an additional pressure gradient in the particle phase momentum equation. If the granular phase packing limit is approached, the additional gradient in the phase momentum equation becomes very large. This should block the increase in the solid volume fraction and lead to a redistribution of the particle phase in the zones where the volume fraction is lower. However, the rapid increase in the additional pressure gradient often results in unstable behaviour in the numerical solution of the two-fluid model.

Syamlal (1998) proposed sensitising the equation for the particle phase volume fraction to the granular pressure derivative $\frac{\partial P_s}{\partial \alpha_s}$, obtaining a correction equation for the volume fraction. This additional equation is solved numerically after the gas flow field is calculated and selective under-relaxation is applied to the volume fraction, where its value becomes close to the packing limit, in order to avoid instabilities. The solids velocity is then calculated on the basis of the corrected volume fraction.

Chen et al. (2003) developed an a posteriori procedure based on the calculation of the contact force required to keep the solids volume fraction under its maximum value in a given computational cell. In this approach, if the packing limit is exceeded, the volume fraction is locally reset to its maximum value, the particle pressure required to maintain this condition is calculated using an iterative procedure and it is imposed on the cell faces.

Lettieri et al. (2003) proposed an explicit a posteriori correction method for two-dimensional uniform grids with cells of equal size, which acts after the completion of each single time step iteration of the solution process. After the flow and the volume fraction fields are calculated at a given time step, the excess of solid particles in a cell is equally redistributed among the adjacent cells by applying the correction given by equation (1), which is clarified in figure 1.

\[
\alpha_{s,(i,j)}^{\text{new}} = \alpha_{s,(i,j)}^{\text{old}} - \alpha_{s,(i,j)}^{\text{ex}} + \frac{1}{4} \left[ \alpha_{s,(i-1,j)}^{\text{ex}} + \alpha_{s,(i+1,j)}^{\text{ex}} + \alpha_{s,(i,j-1)}^{\text{ex}} + \alpha_{s,(i,j+1)}^{\text{ex}} \right]
\]  

Cammarata et al. (2003) extended this approach to three-dimensional computational grids with cells of equal size. Lettieri (2006) extended the method to stretched hexahedral grids in order to simulate narrow fluidised beds.

The aim of this work is to generalise the method proposed by Lettieri et al. (2003), Cammarata et al. (2003) to grids made of cells with different shapes and sizes, and to validate it through the simulation of dense gas-solid fluidised beds. This is necessary to make the method suitable for the simulation of complex geometry systems, where non-uniform and unstructured grids are required.

2 DESCRIPTION OF THE PROCEDURE

The Lettieri et al. (2003) procedure can be extended to general non-uniform and unstructured grids considering that the increase in the concentration of solid particles in the cells adjacent to an over-packed cell should be equal for each cell, in order to uniformly redistribute the solids excess. This can be achieved by weighting the excess of solid...
particles distributed among the adjacent cells on a volume basis. To clarify this concept, the situation in figure 2 can be considered, where cell number one is supposed to be over-packed, with an excess volume fraction $\alpha_{s,1}^{ex} = \alpha_{s,1} - \alpha_{s,max}$. In this case, the redistribution of particles can be performed through equation (2). $V_{n,j}$ represents the sum of the volumes of the cells neighbouring to cell $j$.

$$\alpha_{s,1}^{new} = \alpha_{s,1}^{old} - \alpha_{s,1}^{ex} + \frac{\alpha_{s,2}^{ex} V_1}{V_{n,2}} + \frac{\alpha_{s,3}^{ex} V_1}{V_{n,3}} + \frac{\alpha_{s,4}^{ex} V_1}{V_{n,4}} + \frac{\alpha_{s,5}^{ex} V_1}{V_{n,5}}$$

(2)

Equation (2) is re-written in general form as shown in equation (3), which refers to an over-packed cell $i$.

$$\alpha_{s,i}^{new} = \alpha_{s,i}^{old} - \alpha_{s,i}^{ex} + \sum_{j \neq i} \frac{\alpha_{s,j}^{ex} V_i}{V_{n,j}}$$

(3)
Equation (3) obviously reduces to equation (1), if the grid is made of squared or rectangular cells with the same volume.

It is important to notice that the general formulation of the algorithm shown in equation (3) is valid for all the cells of the computational domain, while equation (1) is not valid for cells adjacent to a wall or to a boundary, for which special conditions have to be developed (Lettieri et al., 2003).

3 IMPLEMENTATION OF THE ALGORITHM

The generalised excess solids volume correction method of equation (3) was implemented in OpenFOAM (OpenCFD, 2005a,b), which allows an easy manipulation of the vectorial and scalar fields, and an easy access to the structure of the computational grid. This permitted the greatest difficulty to be overcome concerning the implementation of the method in its generalised form, which consists in quickly finding the adjacent cells to a given one.

4 VALIDATION OF THE ALGORITHM

The algorithm was validated through the simulation of a fluidised bed \((D=0.15m, H=1m)\) where the superficial gas velocity was reduced one thousand times under the minimum fluidisation velocity: \(u_g=0.001u_{mf}\) (Chen et al., 2003). The solid particles considered in the simulations have a density \(\rho_s=2500\, kg/m^3\) and a diameter \(d_p=300\, \mu m\). The bed was supposed to be in a uniformly expanded state at the beginning of the calculation, with an initial volume fraction of the particle phase equal to 0.55. The value of the packing limit was set at 0.65.

The simulation was performed on a uniform hexahedral grid and on an unstructured tetrahedral grid, both with a cell edge length of 5 mm. The results of the two calculations were compared to verify whether the extended algorithm provides, on unstructured grids, the same results as the original one, applied to structured meshes.

5 THE MATHEMATICAL MODEL

The fluidised bed considered in this work was simulated using a Eulerian-Eulerian two-fluid model. In this approach, the gas phase and the granular phase are treated as interpenetrating continua, solving a continuity and a momentum equation for both of them. Coupling is achieved through a momentum exchange term related to the drag, which was modelled according to Gidaspow (1994). All other interactions between the phases were neglected in the calculations, as well as the gas turbulence.

The simulations presented in this paper are only a test case for the algorithm to enforce the packing limit, therefore, for simplicity, the particle phase was described as a fluid with constant viscosity (Gidaspow, 1994).

5.1 Boundary conditions

The velocity of both phases were imposed at the inlet of the bed, where all other variables were supposed to have uniform profiles. The pressure was set to the atmospheric at the outlet. No-slip boundary conditions were set at the walls, for either phase. Neumann conditions were adopted for all the other variables at the wall and at the outlet.

6 NUMERICAL SOLUTION PROCEDURE

The equations of the two-fluid model were solved using OpenFOAM. The coupling between the pressure and velocity is obtained through the Pressure Implicit with Splitting of Operators (PISO) algorithm proposed by Issa (1986).
momentum equation was solved in its phase-intensive form, according to Weller (2002) and Rusche (2002), while the phase continuity equation was solved in the form proposed by Weller (2002), in order to bind the phase volume fraction between zero and one. A TVD limited version of the central difference scheme, was used for the discretisation of the convective terms of all equations, with the exception of the phase continuity equation, for which the same scheme was adopted in a bound fashion. Two PISO corrector steps and two iterations for non-orthogonal correction were performed, as well as two correction iterations for the continuity equations.

The systems of linear equations obtained through the discretisation of the transport equations were solved using the conjugate gradient method with incomplete Cholesky preconditioning (Jacobs, 1980) for the pressure equation, while the bi-conjugate gradient method (Van Der Vost, 1992) was adopted for all other equations. Tolerances were set to $1.0 \cdot 10^{-10}$ for the pressure, and to $1.0 \cdot 10^{-5}$ for all the other variables. A time step of $1.0 \cdot 10^{-5}$ s was used to obtain accurate results.

7 RESULTS

The results of the two simulations discussed in §4 are reported in figure 3, which shows the evolution in time of the particle phase volume fraction on the structured hexahedral grid (a) and on the unstructured tetrahedral grid (b). In both calculations, the solid particles continue to accumulate on the bottom of the bed, as a consequence of gravity, until the value of the solids volume fraction reaches its maximum, equal to the expected value for $\alpha_{s,max}$, which is never surpassed. The slight difference at the freeboard of the bed, which appears to be less sharp in (b), is a consequence of the adoption of the tetrahedral grid, which is less capable of capturing sharp interfaces than hexahedral discretisation.

8 CONCLUSIONS

The excess solids volume correction method proposed by Lettieri et al. (2003), Cammarata et al. (2003) to enforce the particle phase packing limit in two-fluid simulations has been extended to unstructured grids.

Figure 3. Time evolution of the particle phase volume fraction with the packing limit algorithm on (a) the hexahedral and on (b) the tetrahedral grid.
The proposed extension was implemented in OpenFOAM and validated by comparing the results of the simulation of a fluidised bed, in which the gas feed velocity was reduced to less than the minimum fluidisation velocity, both on structured and unstructured grids. The algorithm has proved to be capable of avoiding the particle phase over-packing, without altering the physical behaviour of the system.

The effectiveness of the procedure and its capability to not alter the solution is closely connected to the time step size, as already stated by Lettieri et al. (2003). Smaller time steps grant small changes in the solution at each step. Consequently only a few cells result to be overpacked at each time step and require correction.

ACKNOWLEDGMENTS

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NOTATION

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$D$</td>
<td>Diameter of the fluidised bed, m</td>
</tr>
<tr>
<td>$H$</td>
<td>Height of the fluidised bed, m</td>
</tr>
<tr>
<td>$P_s$</td>
<td>Particle phase pressure, Pa</td>
</tr>
<tr>
<td>$u_g$</td>
<td>Gas phase velocity, m/s</td>
</tr>
<tr>
<td>$u_{mf}$</td>
<td>Minimum fluidisation velocity, m/s</td>
</tr>
<tr>
<td>$V_i$</td>
<td>Volume of the cell, m$^3$</td>
</tr>
</tbody>
</table>

Greek letters

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{s,max}$</td>
<td>Particles packing limit</td>
</tr>
<tr>
<td>$\alpha_s$</td>
<td>Particle phase volume fraction</td>
</tr>
<tr>
<td>$\alpha_{ex}$</td>
<td>Excess volume fraction of the particle phase</td>
</tr>
<tr>
<td>$\rho_i$</td>
<td>Density of the phase i, kg/m$^3$</td>
</tr>
</tbody>
</table>

REFERENCES


