THE EFFECT OF NUMERICAL DIFFUSION ON GAS-SOLIDS FLUIDIZED BEDS
AND THE USE OF DEFERRED CORRECTION IN A FINITE VOLUME METHOD
TO STABILIZE HIGH ORDER DISCRETIZATION OF CONVECTION TERMS

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Abstract. First order methods are commonly used in numerical simulations of gas-solids fluidized beds because they are both stable and affordable. Unfortunately, because of the large amounts of numerical diffusion inherent to these methods higher order methods are recommended to accurately predict bed dynamics e.g., voids or bubbles. The deferred correction method and the downwind factor method are both used for generating linear equations based on a 7-point stencil from higher order discretization formulas. Deferred correction significantly improves the computational speed over the downwind factor method while achieving the same degree of accuracy and under certain conditions allowed computations which the downwind factor method failed.

Key words. Fluidization; convection; diffusion; bubbles; deferred correction

AMS subject classifications. 74S10, 76T25, 76M12

1. Introduction. Gas-solids fluidized beds are used in many industrial applications to drive chemical or combustion/gasification processes. To identify process modifications which will improve the reactor performance, industry increasingly relies upon numerical simulations of fluidized bed reactors. A distinct feature of gas-solids fluidized beds is the bubbles (regions with very little or no solids), which significantly affect reactor performance by maintaining uniform bed temperature on the one hand, while allowing reactant bypassing on the other hand. So it is essential to understand their characteristics and transient behavior.

This paper uses a two-fluid model in which the gas and the solids are considered to be interpenetrating continua and their flow is calculated by a set of mass and momentum balance equations. An additional field variable void fraction is needed in such a formulation to account for the fraction of the volume occupied by gas. The stresses in the solids phase is determined from kinetic theory of granular flow [1]-[3].

The idea of describing fluidized beds with two-fluid hydrodynamic models have existed since the early 60’s while numerical solutions that predict bubbles came much later [4]-[8]. In each of these studies, predicted bubble shapes, observed from contour plots of void fraction, produced pointed and elongated bubbles rather than the typical rounded kidney shape bubbles found experimentally. These studies raised the question whether the two-fluid model is incomplete in some manner as to result in the prediction of unphysical bubble shapes or whether the numerical technique used was inadequate to solve the equations correctly.

The first objective of this paper is to demonstrate that two-fluid models can be solved using a finite volume method to calculate physically realistic bubble shapes. This paper will show that the pointed bubble shape is a numerical artifact resulting from the use of first order upwinding (FOU) for discretizing convection terms while second order methods such as Superbee, SMART, and MINMOD produce physically realistic rounded shape. Details on how numerical diffusion influences the predicted shape of a bubble is included in this investigation.

A second objective of this paper is to compare two methods for implementing higher-order discretization schemes into two-fluid codes: the downwind factor method (DWF) pro-
posed by [9] and the deferred correction method (DC) of [10]. Higher order discretization schemes use information from a wider stencil than a 7-point stencil (in 3D). The DWF and DC methods use techniques used to generate linear equations based on a 7-point stencil from higher order discretization formulas. In the DWF method quantities defined at control volume faces are calculated in terms of their DWF’s and adjacent upstream and downstream nodal values. This keeps a compact structure to the resulting system of discretized equations with the contribution of a wider stencil and the non-oscillatory universal limiter constraints [9] implicitly contained in the DWF. The expectation was that this technique would guarantee non-oscillatory results with the stability and convergence properties of FOU. Unfortunately, under certain conditions DWF method leads to instabilities because of the emphasis placed on downstream nodal values rather than upstream nodal values [11]. The DWF method can destroy the diagonally dominant structure of the coefficient matrix and slow convergence rates or in some cases leads to divergence.

The DC method keeps the algebraic structure of low order methods by the addition of a source term which contains the difference between the low and high order methods. This somewhat older technique is no longer preferred in single phase calculations because the source term places an undue burden on convergence. The performance of this technique in gas-solids flow calculations has not been reported. This paper will show that DC is an effective method for gas-solids calculations. The main reason for this is that gas-solids calculations are inherently transient and need fairly small time steps. So the magnitude of the source term created by DC method is usually small in gas-solids flow calculations and does not adversely affect convergence. Because DC uses a low order method (FOU) in the formation of the algebraic system a diagonal dominant system is generated. This increased stability afforded by the DC method significantly improves computational speed in comparison to DWF method while achieving the same degree of accuracy.

Another advantage of the DC method demonstrated in this paper is the use of DC to implement very high order discretization schemes into two-fluid models. This paper extends the recent work of [12] to the two-fluid model used in this investigation. Results show very good agreement with experimental data [8].

2. Hydrodynamic Model. The code used to solve the standard two-fluid model is MFIX(Multiphase Flow with Interphase eXchanges) which was developed at the Department of Energy’s National Energy Technology Laboratory [13]. Under isothermal conditions, two phases (gas and solids), and no reactions the continuity and momentum balance equations are given below.

Gas-phase continuity

\[
\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{v}_g) = 0
\]  

(2.1)

Solids-phase continuity

\[
\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla \cdot (\varepsilon_s \rho_s \vec{v}_s) = 0
\]

(2.2)

Gas-phase momentum

\[
\frac{\partial}{\partial t}(\varepsilon_g \rho_g \vec{v}_g) + \nabla \cdot (\varepsilon_g \rho_g \vec{v}_g \vec{v}_g) = -\varepsilon_g \nabla P_g + \nabla \cdot \vec{T}_g + \vec{F}_{gs}(\vec{v}_s - \vec{v}_g) + \varepsilon_g \rho_g \vec{g}
\]

(2.3)
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Solids-phase momentum

\[
\frac{\partial}{\partial t}(\varepsilon_s \rho_s v_s) + \nabla \cdot (\varepsilon_s \rho_s v_s \vec{v}_s) = -\varepsilon_s \nabla P_s - \nabla \cdot \vec{T}_s - F_{gs}(\vec{v}_s - \vec{v}_g) + \varepsilon_s \rho_s \vec{g}
\]

Expressions for the gas-phase stress $\vec{T}_g$, gas-solids drag $F_{gs}$, granular stress $\vec{T}_s$, and solids pressure $P_s$ are needed to close the system. Constitutive models for these variables can be found in [13] and [14].

3. Numerical Procedure. A sequential iterative procedure is used to solve (2.1)-(2.4) that begins with a finite volume method on a staggered grid. The partial elimination algorithm [15] decouples the momentum equations and an extension of SIMPLE [16] is used to adjust velocities in order to satisfy conservation of mass. A solids volume fraction correction equation updates the solids volume fraction which is used to update the solids velocity field and the solids pressure. Convergence is then determined by the calculated residuals from the velocity and pressure equations of both phases.

Because we are only concerned about the discretization of convection terms in this paper, we will use the general property balance equation given by

\[
\frac{\partial}{\partial t}(\varepsilon_m \rho_m \phi) + \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m v_m \phi) = \frac{\partial}{\partial x_i} \left( \Gamma \frac{\partial \phi}{\partial x_i} \right) + R_{\phi}.
\]

Equation (3.1) is the transport equation for a scalar property $\phi$ of the gas phase $m = g$ or the solids phase $m = s$. The terms in (3.1) represent rate of change, convection and diffusion effects, and a source term $R_{\phi}$ for the quantity $\phi$. In multi-phase flows the source term accounts for interphase mass and momentum transfer. Since the relevant features of (2.1)-(2.4) are contained in the transport equation, (3.1) will be used in the next sections to introduce the discretization techniques used in this paper.

3.1. Finite Volume Method. The finite volume method begins by formally integrating (3.1) over an arbitrary control volume. Using standard compass point notation about the nodal point $P$ expressions for the transient, convection, and diffusion terms are given by the following expression:

\[
\int_{CV} \frac{\partial}{\partial t}(\varepsilon_m \rho_m \phi) dV \approx \left[ (\varepsilon_m \rho_m \phi)_p - (\varepsilon_m \rho_m \phi)_p^{old} \right] \Delta V / \Delta t.
\]

\[
\int_{CV} \frac{\partial}{\partial x_i}(\varepsilon_m \rho_m v_m \phi) dV \approx (\varepsilon_m \rho_m \phi)_e(v_m)_e A_e - (\varepsilon_m \rho_m \phi)_w(v_m)_w A_w
\]

\[
+ (\varepsilon_m \rho_m \phi)_n(v_m)_n A_n - (\varepsilon_m \rho_m \phi)_s(v_m)_s A_s
\]

\[
(3.3)
\]

where $A$ is the cross-sectional area of the control volume and $t, b$ are the top and bottom of a cell face.

\[
\int_{CV} \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) dV \approx \left( \Gamma \frac{\partial \phi}{\partial x_j} \right)_e A_e - \left( \Gamma \frac{\partial \phi}{\partial x_j} \right)_w A_w
\]

\[
+ \left( \Gamma \frac{\partial \phi}{\partial y} \right)_n A_n - \left( \Gamma \frac{\partial \phi}{\partial y} \right)_s A_s
\]

\[
+ \left( \Gamma \frac{\partial \phi}{\partial z} \right)_t A_t - \left( \Gamma \frac{\partial \phi}{\partial z} \right)_b A_b
\]

(3.4)
Equations (3.3) and (3.4) represent the convective and diffusive fluxes across the faces of a control volume. The diffusive flux is approximated by a simple interpolation scheme which is easily shown to be accurate to second order. For example, the diffusive flux at the east face is given by

\[
\left( \Gamma \frac{\partial \phi}{\partial x} \right)_e = \left( \Gamma \frac{\partial \phi}{\partial x} \right)_e \frac{\phi_E - \phi_P}{\Delta x_e} + O(\Delta x^2).
\]

The discretization of the convection term is a crucial task and is the main topic of this paper. Evaluation of the convection term requires an expression for \( \phi \) at each face of a cell. The widely used method in gas-solids flow calculations is FOU, which although stable is only first order accurate and, hence, highly diffusive. Higher-order discretization techniques, on the other hand, produce unphysical oscillations in solution that can slow down or destroy convergence. A remedy for the numerical oscillations is to apply a flux limiter. Leonard and Mokhtari [9] introduced a universal limiter that can be expressed as a function of a normalized value of \( \phi \) defined as

\[
\tilde{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U}
\]

where the subscripts \( U \) and \( D \) represent upstream and downstream nodes based on flow direction.

3.2. Downwind Factor Method. The universal limiter can be expressed in terms of downwind weighting factors [9] to generate an implicit compact stencil suitable for tridiagonal (or septadiagonal in 3D) solution methods. The DWF is defined as

\[
DWF = \frac{\phi_f - \phi_C}{\phi_D - \phi_C} = \frac{\hat{\phi}_f - \hat{\phi}_C}{1 - \hat{\phi}_C}
\]

where \( C \) is a node between \( U \) and \( D \). Leonard and Mokhtari [9] describes a procedure for applying the limiter to any arbitrary higher order scheme. In practice, explicit formulas for the DWF’s can be obtained by evaluating \( \frac{\phi_f - \phi_C}{\phi_D - \phi_C} \), where \( \phi_f \) is replaced by its interpolated value. Once the DWF has been determined it is clear that the cell face value, \( \phi_f \), is given by

\[
\phi_f = DWF \phi_D + (1 - DWF) \phi_C.
\]

Equation (3.8) can be converted into compass point notation by introducing a convection weighting factor \( \xi \) defined as

\[
\xi_u = \begin{cases} 
DWF & u \geq 0, \\
1 - DWF & u < 0.
\end{cases}
\]

The value of \( \phi \) at the east face, for example, is then written as

\[
\phi_e = \xi_E \phi_E + \xi_P \phi_P
\]

where \( \xi_e = 1 - \xi_e \). Using the above expressions for the term \( \epsilon_m \rho_m \phi \) in the right hand side of (3.3) along with the expressions for the transient and diffusion terms results in the following linear system

\[
a_p \phi_p = \sum_{nb} a_{nb} \phi_{nb} + S_p
\]

where \( S_p \) is the contributions from the discretization of the transient term and the volume integral of the linearized source term, the subscript \( nb \) represent contributions from the E, W, N, S, T, and B faces of the cell.
3.3. Deferred Correction Method. As an alternative to DWF method the deferred correction (DC) method [10] was implemented into MFIX. Deferred correction uses the desirable stability properties of a low order method, in this paper FOU, to form the algebraic system given by (3.11). To capture the resolution of a higher order method an additional source term is added

\[
a_P \phi_P = \sum_{nb} a_{PL} \phi_{nb} + S_P + S_{DC}.
\]

The additional source term is given by

\[
S_{DC} = (\epsilon_m \rho_m) f(v_f) (\phi^{LO} - \phi^{HO}) A_f.
\]

Equation (3.12) is derived by adding and subtracting FOU convection terms to the higher order convection terms. The higher order convection terms and the subtracted out FOU convection terms are combined to form the source term \(S_{DC}\). The added FOU convection term appears implicitly in the coefficients \(a_P\) and \(a_{PL}\). Since the added and subtracted FOU convection term cancell out, at convergence there is no net contribution to equation (3.12) from \(\phi^{LO}\). Therefore, at convergence the discretization used in equation (3.12) is purely higher order.

4. Numerical Results. Results given in this section represent the numerical solution of (2.1)-(2.4) using the techniques presented in preceeding section. The limited second-order schemes were used for all the convection terms appearing in equations (2.1)-(2.4). The value of different variables at the control volume faces is calculated by substituting \(\epsilon_g \rho_g\) and \(\epsilon_s \rho_s\) for \(\phi\) in equation (3.10). Similarly, \((v_g)\) and \((v_s)\) are substituted for \(\phi\) in an obvious extension of equation (3.10) for staggered grids. Details on the treatment of the individual terms found in (2.1)-(2.4) and the algebraic manipulation required to produce a discretized system of equations of the form given by (3.11) can be found in [14].

4.1. Fluidized Bed Simulations. The computational region is 39.37 cm wide by 58.44 cm high. The initial bed height is 29.22 cm with a initial void fraction, \(\epsilon_g = 0.44\). The particles have a uniform diameter of 500 \(\mu\)m and a density of 2660 kg/m\(^3\). Air enters the bottom of the bed with a velocity of 23.4 cm/s maintaining the bed at minimum fluidization. A jet of width 1.5 cm is centrally located at the bottom of the bed. Initially, air enters through the jet with a flow rate identical to the minimum fluidization velocity. At \(t=0.13\)s, the velocity at the jet is increased to 520 cm/s, which is sufficient to form a bubble or void in the bed. The physical parameters given above are taken from [8] and correspond to a classical fluidization experiment described by [6]. The full two-dimensional bed was simulated without assuming symmetry. No-slip condition was imposed on the two side walls.

The spatial mesh used was 124 computational cells in the \(x\)-direction and 108 cells in the \(y\)-direction and was based on the grid independent results established during the course of this investigation. Figure 4.1 shows the shape of a bubble predicted by the first order method FOU. The bubble is given by a contour plot of the void fraction, in this paper the value is \(\epsilon_g = 0.37\). The solution is given at times \(t=0.36\)s, \(t=0.59\)s, and just prior to the bubble reaching the surface \(t=0.66\)s. The shape of the bubble as it detaches and rises through the bed agrees closely with the results found in earlier investigations \(e.g.\) [6] and [7]. Note the unphysical pointed shape of the bubble. In Figures 4.2 and 4.3 the results are obtained from the second order schemes: MINMOD and Superbee using DC and the same mesh size and contour concentration level as the FOU case. The results of the SMART scheme are very similar to the Superbee scheme and are not shown. The shape of the bubble during its formation and rise using the DWF method are very similar to the DC results and are not shown. The results
are given at the same times except for the time prior to the bubble reaching the surface. In each of these cases a rounded bubble forms at the jet which detaches and travels up through the bed.

![Fig. 4.1. Bubble Formation and Rise Using First Order Upwinding.](image)

**4.2. Numerical Diffusion.** The different shapes given in Figures 4.1-4.3 are attributed to the different amounts of diffusion introduced by the discretization of the convective terms. It is somewhat counter intuitive to expect that the scheme with the largest amount of numerical diffusion (FOU) produces bubbles which are pointed. To explain why pointed bubbles are observed numerical experiments were performed which showed a pointed or rounded shape bubble was completely determined by the type of discretization scheme used in the solids momentum equation. These results showed that when a higher order scheme was used to discretize the convective terms in the solids momentum equation and FOU was used in the gas and solids continuity equations and the gas momentum equation the result was a rounded bubble shape. Alternatively, when FOU was used in the solids momentum equation and a higher order method was used in the other equations the result was a pointed bubble. The fact that the bubble shape depends on the type of discretization scheme used in the solids momentum equation is because of the different solids velocity profiles predicted by FOU and a higher order method. Across any horizontal plane in the bed FOU and a higher order method predict a solids velocity profile which is parabolic because of numerical diffusion in the solids momentum equation. However, near the tip of the bubble FOU predicts a higher solids velocity than any of the other higher order methods considered. This produces larger convection at the center of the jet causing the void fraction to be swept farther downstream resulting in a pointed shape bubble. Conversely, the flatter velocity profile predicted by a higher order scheme such as Superbee or SMART resulted in a rounded bubble. Although it is formally second order, MINMOD predicts a more of an elliptic shape than Superbee (Figure 4.2). This result is not surprising since MINMOD can be shown to be more diffusive than either Superbee or SMART. Not only do these results show how numerical diffusion affects the shape of a bubble they also demonstrate how numerical diffusion can prevent the prediction of surface instabilities like the one shown in Figure 4.3. These instabilities are caused by solids raining down through the top of the bubble which can produce irregularities in the profile of the bubble and can significantly affect bed dynamics. Surface instabilities like the one predicted by Superbee often cause the bubble to split into smaller bubbles. These bubbles then tend to coalesce into each other further complicating the dynamics of the bed. Similar phenomena have been observed experimentally by [6] and [8].

**4.3. Very High Order Methods.** A very nice feature of the linear system given by (3.12) is the fact that the added source term \( S_{DC} \) is evaluated explicitly. That is, the nodal points at the current iteration level are used to evaluate \( \phi^{LO} \) and \( \phi^{HO} \). This feature does not
restrict the DC method to just second order schemes. Very high order schemes which generally require large stencils can now be implemented explicitly. The upwind biased fourth order method of [12] was used in this investigation. This scheme approximates convective fluxes with a four-point fourth order interpolation (FPFOI) scheme. The results presented in [12] did not require any type of limiter to suppress numerical oscillations. However, implementation of this scheme into MFIX required the use of the universal limiter [9] because of the sensitivity of the solids phase. Single phase (gas only) calculations did not require any limiter. To demonstrate the effectiveness of using very high order discretization schemes to approximate convective fluxes the experiments of [8] were used. These experiments are very similar to the ones considered earlier. These experiments used a 2-d fluidized bed 57 cm wide and 100 cm high. The particles used in these experiments are the same used earlier. A central jet operating at 1000 cm/s is used. Results shown in Figure 4.4 is the solids volume fraction time-averaged over 60 seconds of data along vertical planes 0.4 cm and 3.4 cm from the center of the bed. These results agree closely with the experimental data and show a significant improvement over the Superbee method. Finally, Both FPFOI and Superbee predicted qualitatively similar bubbles and the computational time required for the FPFOI method was similar to that of the Superbee scheme.

4.4. CPU Comparison. Table 4.1 compares the computational time required by DWF method and DC method for the results given by Figures 4.2, 4.3, and the SMART scheme with two different jet velocities (520 cm/s and 1000 cm/s). The cpu times are given in seconds and are recorded between the times t=0.79s and t=1.0s. These times were selected because initially the jet is operating at minimum fluidization velocity, its effect on the bed is very small, and very little difference is observed between DWF and DC methods. At later times the entire bed is in a highly transient state and the faster computational times due to DC are easily observed. These results show that DC method can significantly improve computational times when higher order methods are used in the discretization of the convective terms. In
5. Conclusion. We have investigated the effects of numerical diffusion on the formation of bubbles in a gas-solids fluidized bed. We have shown the formation of pointed bubbles is due to numerical diffusion introduced by FOU in the approximation of convective terms in the solids momentum equation. Higher order methods such as Superbee, SMART, and FP-FOI produced physically realistic rounded bubbles. Higher order methods, including FPFOI, predicted instabilities on the surface of a bubble which was not evident using FOU.

Because DC uses FOU in the formation of the algebraic system a diagonal dominant system is generated. This increased stability afforded by the DC method significantly improved computational speed in comparison to the DWF method while achieving the same degree of accuracy. In gas-solids flow computations we find that the use of DC method improves the computational speed by an average of 30%. The DC method was also shown to provide a convenient platform to implement very high order discretization schemes into two-fluid models. These results further demonstrate the importance of using high order schemes in the approximation of convective fluxes.

REFERENCES

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