Numerical models of fluidized beds based on the multiphase mass and momentum balance equations for gas and solids phases [1] continue to be developed by several groups of researchers around the world. It has been demonstrated that the same set of equations is able to describe a wide range of fluidization conditions, ranging from bubbling to circulating fluidized beds [1].

The results of bubbling bed simulations, plots of void fraction distribution, show the formation and propagation of high void-fraction regions, called bubbles. Bubble characteristics such as the rise velocity, wake angle, void fraction distribution, and pressure distribution have been compared with experimental data [e.g., 1, 2]. It has been shown that the simulations qualitatively predict experimentally observed solids movement in the bubble wake and *slow* and *fast* bubbles [2].

The predicted bubble shapes observed from contour plots of void fraction differ from experimental observations in one peculiar manner: the nose of the calculated bubble is pointed unlike the rounded shape of experimental bubbles. This problem appears in the simulation results published by various authors using different computational techniques [1, 2, 3, 4, 5]. Another disagreement with experimental observations is that simulations with a continuous jet predict the formation of a permanent "fountain" of solids at the bed surface, much like a spouting bed [6]. To get physically realistic predictions, researchers have attempted to modify the theory. This study shows that these problems are numerical artifacts of using first order accurate discretization schemes and coarse grids and are not due to a fundamental difficulty with the theory.

An implication that the theory can be expected to predict rounded bubbles comes from the numerical simulations based on distinct element models (DEM) [7]. In a DEM model of fluidization developed by Tsuji and coworkers the motion of individual particles rather than the motion of an averaged solids phase is calculated. Gera and Tsuji showed that the DEM model predicted rounded bubble shape, whereas a multiphase model, under identical conditions, predicted a pointed bubble. This comparison implies that the pointed shape is perhaps a numerical artifact, since the solids momentum equation in the multiphase model is a reasonable average of the particle trajectory equations in the DEM model.

The above conjecture was clearly substantiated by Sokolichin et al. in a study of gas-liquid two phase flow [8]. They compared a multiphase model with a Lagrangian particle tracking model and as in [7]
DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.
found that the Lagrangian particle tracking model gave a rounded profile of the gas holdup, where as the multiphase flow model yielded a pointed gas holdup profile. They then showed that the multiphase flow model can predict a rounded profile that agrees with the profile calculated with the Lagrangian particle tracking model when the first order upwind (FOU) scheme used in the multiphase flow model is replaced with a second order accurate discretization scheme. The pointed shape is a result of the large numerical viscosity of the FOU scheme, which is of the order of \((U\Delta x/2)\), where \(U\) is the velocity and \(\Delta x\) is the grid size. At first it appears counterintuitive that a diffusion effect would make the profile pointed rather than rounded. Sokolichin et al. point out that this so because of the directional dependence of numerical diffusion: the vertical component of velocity is much greater than the radial component, and, therefore, the axial diffusion is much greater than the radial diffusion.

Christie et al. calculated an unpointed, but very unphysical bubble shape, with the FOU scheme. With the use of a second order accurate scheme they could predict rounded bubble shapes [10]. The results of first order upwind scheme and several second order schemes were compared in [11]. The second order methods gave sharper bubble boundaries, but no conclusions were drawn regarding bubble shape.

This study was motivated by the observation that the shape of the gas hold up profile described by Sokolichin et al. [7] is similar to that of the shape of bubbles in a fluidized bed. Second-order accurate discretization schemes were included in a multiphase flow model of fluidized beds called MFIX [9]. It is shown here that the bubble shape predicted with a second order accurate scheme is rounded. The simulations were conducted for long durations (5 s) and the results did not show the fountain formation at the bed surface. It appears that the fountain formation is caused by coarse grids and low physical viscosity of the solids phase.

**DISCRETIZATION METHODS**

Fluidized beds are convection-dominated flows, and the convection terms must be discretized accurately. The use FOU scheme for discretizing the convection terms leads to a stable but diffusive set of difference equations. Second and higher order methods, although formally more accurate than FOU, produce spurious oscillations in the solution. To eliminate the spurious oscillations while maintaining higher order accuracy, a limiter is applied to the discretization scheme [12]. Second order accurate schemes Superbee, Smart, Muscl, van Leer, and Minmod and the third order accurate method Ultra-quick, were added to MFIX. The down wind factor approach discussed in [12] was used for converting the higher order differences into the septa diagonal matrix structure used by MFIX linear equation solver.

**TESTING OF DISCRETIZATION METHODS**

Figure 1 shows a comparison of a moving plug problem simulated with MFIX to test the various discretization schemes. In this simulation only the solids continuity equation was solved. For clarity, the exact solution and only the solutions obtained with Superbee, Smart and FOU schemes are shown in the figure. At time zero the plug occupies the distance 80-90 cm and moves at a steady velocity of 5 cm/s in the negative x-direction. Figure 1 shows the predictions at 10 s. The FOU and Smart schemes give a smeared, smooth profile. The FOU scheme smears the profile to such an extent that even the peak solids volume fraction is less than 60% of the actual value. The Superbee scheme calculates the exact peak value and nearly reproduces the discontinuity. Ultra-quick results, not shown in the figure,
were not distinguishable from the Superbee results. The Minmod and van Leer schemes gave nearly identical results that fell somewhere between FOU and Smart results.

A comparison of the normalized CPU times for this simulation is made in Table I. The table shows that Smart is the least expensive second order method and Ultra-quick is the cheaper of the two most accurate schemes. When the full set of equations was solved to simulate a bubbling fluidized bed, however, getting a stable solution with Ultra-quick was not possible. Also, the CPU time ratio for Superbee to FOU decreased to a factor of only 1.14. This considerable reduction is perhaps because the ratio of number of computational cells resolving the sharp gradients to the total number of cells is smaller in the bubbling bed simulation than in the moving plug simulation. Therefore, in the subsequent simulations Superbee was used as the higher order method of choice, as it gave the most rounded bubble shape.

Table I. Normalized CPU time requirements for the moving plug problem

<table>
<thead>
<tr>
<th></th>
<th>FOU</th>
<th>Smart</th>
<th>van Leer</th>
<th>MinMod</th>
<th>Ultra-Quick</th>
<th>Superbee</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>4</td>
<td>5</td>
<td>9</td>
<td>43</td>
<td>81</td>
</tr>
</tbody>
</table>

BUBBLING FLUIDIZED BED WITH A CENTRAL JET

The bubbling fluidized bed experiments of Gidaspow [1, pp. 156-158] with a central jet were simulated. MFIx equations [9] with Gidaspow's drag correlation [1, p. 151] were solved. No symmetry was assumed and a 128x104 cell distribution was used. Figure 2 shows the calculated void fraction ($\epsilon$) distribution in the 500 µm particle bed with a 3.55 m/s jet: white - $\epsilon > 0.9$, light gray - $0.7 < \epsilon < 0.9$, dark gray - $\epsilon < 0.7$. In these two simulations the solids viscosity was first set to zero. The first bubble as it is ready to detach is shown on the left-hand-side. The nose of the bubble predicted with Superbee is rounded and that of FOU is pointed. With Superbee scheme the bubbles appeared realistic during the first 1 s. After 1 s, the bed became freely bubbling. Some bubbles even moved downwards. A similar loss of bubbling is discussed in [5]. With FOU scheme reasonable behavior lasted up to 2.5 s, and afterwards the bed became freely bubbling (left panels of Fig. 2). The FOU scheme predicts central bubbling for a longer time because of the inherent numerical viscosity.

By turning on the frictional regime stress formulation in MFIx, a stable, centrally bubbling pattern was predicted as seen in experiments (Figure 3). Usually both schemes predict a sharp lower boundary for the bubbles, as shown by the absence of light gray regions near the lower boundary, and a diffused
upper boundary [11]. In Fig 3 the lower boundaries of the bubbles predicted with Superbee, however, have light gray regions because of recent bubble coalescences. The bubbles predicted with Superbee scheme have a much sharper boundary than that predicted with FOU and are round shaped. Bubbles being captured in the wake of another bubble, however, become elongated. The rounded bubbles were slightly slower than the pointed bubbles and less frequent (frequency: FOU - 5 Hz; Superbee - 4.3 Hz).

Figure 4 shows the simulation results for 800 μm particles and a jet velocity of 5.77 m/s. The comparison between FOU and Superbee schemes show that Superbee scheme predicts a sharper, rounded bubble. The bubble frequencies were comparable: FOU - 7 Hz; Superbee - 6.7 Hz.

Figure 5 shows the void fraction distributions for jet velocities of 5.77 m/s and 9.88 m/s. These simulations also showed that Superbee scheme gives rounded bubble shapes. At these jet velocities the fluidized bed is more chaotic and bubble shapes deviate from the rounded shape. These predictions qualitatively agree with experimental observations. Figure 5 also shows a phenomenon similar to the raining of solids from the bubble roof often seen in experiments [e.g., 1, p.162]. This effect is more clearly seen in animations of the void fraction distributions.

In Figures 2 - 5 note that a fountain does not form at the bed surface. The fountain formation appears to be an artifact of the poor grid resolution and low physical (solids) viscosity in the previous calculations. This problem is more pronounced with the FOU scheme than with higher order schemes.

CONCLUSIONS

Five second-order accurate discretization methods for convection terms were included in a multiphase flow model of fluidization. Several bubbling fluidized bed simulations were conducted with no stability problems. The study shows that the unphysical “pointed” shape of bubbles is merely a numerical artifact caused by first-order upwind scheme. Simulations with the Superbee scheme predict physically realistic rounded bubbles, and appear to be able to mimic details such as the raining of solids from the bubble roof. The simulations were conducted for long durations (5 s), and the “fountain” artifact [6] was not seen in the results.
LITERATURE CITED


Report Number (14) DOE/FTEC/C-987305
CONF-971113-

Publ. Date (11) 199701

Sponsor Code (18) DOE/FE XF

JC Category (19) UC-101, DOE/ER