Application of coupled solver technology to CFD modeling of multiphase flows with CFX

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Abstract

Over the past ten years the use of Computational Fluid Dynamics (CFD) in chemical engineering has increased at a significant rate. Most of the large chemical engineering companies now use CFD daily in their design process, in problem solving and in improving performance of plants and equipment. The complexity of the problems tackled by CFD is increasing dramatically as the CFD technology advances and is delivered to users in an accessible and user friendly format.

Multiphase flows are involved in almost all of the processes in chemical engineering, for examples: gas bubbles in liquid columns, solid particles in mixing vessels, liquid droplets in spray dryers. Multiphase flow problems are inherently very complex. Many of the physical processes (heat, mass and momentum) are linked and coupled between the phases. Despite the difficulties, many successful CFD calculations have been reported in the literature. In most of the current CFD algorithms for multiphase flows such as Spalding’s IPSA method, a segregated solution method is used. The momentum, continuity and other equations are solved in separate steps. The whole calculation sequence must be iterated many times (typically thousands of iterations) for the solution to address all the coupling terms properly and converge to the final solution.

For single-phase flows, convergence speed can be improved by using what is known as a coupled solver technology. Within this technique the governing transport equations are all solved simultaneously. This strategy has been implemented in CFX-5 to model two-phase flows. In this paper we will describe the coupled solver technology implemented in the CFX-5 software and examine the advances of this technology in terms of CFD performance on a real two-phase example with published experimental data.
1 Introduction

Multiphase flows occur in almost all chemical engineering processes. Examples include:

- Bubble columns.
- Gas-solid and liquid-solid flows in fluidized beds.

The physics of such flows is inherently very complex. This is largely due to inter-phase transfer of heat, mass and momentum, which is typically governed by many distinct physical processes that are only partially understood.

Despite these difficulties, significant progress has been made in the application of CFD to the calculation of such flows. Over the past decade, an extensive multi-phase flow algorithm has been developed in AEA Technology’s CFD solver CFX-4, which models complex geometry using a multi-block structured mesh of hexahedral elements. All variables are co-located at cell centers.

Like most other CFD codes for multiphase flows, CFX-4’s multiphase algorithm is based on Spalding’s IPSA method [1], [5]. This is a segregated method in which the momentum, continuity and other equations are solved in separate steps. This procedure does not perform well on multi-phase flow calculations due to the strong non-linear coupling between equations imposed by inter-phase transfer processes. The calculation sequence must be repeated many times (typically thousands of iterations) for the solution to address all coupling terms properly, and converge to the final solution. Also, the algorithm does not scale well with problem size, with the number of iterations required for convergence typically increasing with problem size.

In parallel with development of advanced models in CFX-4, AEA Technology has also developed its next generation CFD solver, CFX-5. This extends the geometric capabilities of CFX-4 by working with fully unstructured mixed element meshes, including tetrahedral, hexahedral, prismatic and pyramid finite elements. This facilitates the use of automatic mesh generation procedures for use in the initial simulation, and for subsequent automatic refinement. Another major goal in the development of CFX-5 has been the development of a new robust and scalable solution algorithm. This algorithm is built on three foundations:

- Coupled solver technology [2], [4]
- Algebraic multi-grid (AMG) for the solution of large coupled linear systems [2], [4]
- Full parallelization [4].

In the coupled solver, linearized momentum and continuity equations are solved simultaneously for velocity and pressure. This greatly increases robustness, as
much fewer iterations are required to achieve convergence, and much less is required by way of user intervention to achieve convergence. The use of coupled algebraic multi-grid to solve the coupled linear system gives a scalable algorithm in the sense that CPU time increases linearly with problem size. The parallel algorithm uses the Single Program Multiple Data (SPMD) approach and node-based domain decomposition, and is also scalable both in CPU time and memory requirements.

This paper describes the first steps in extending the CFX-5 coupled solver technology to Eulerian-Eulerian multi-phase flows. Our aim is to produce a multi-phase flow algorithm with the same robustness and scalability advantages that have been achieved for single phase flows. This is intended to provide a robust platform for future development of advanced models for complex multi-phase flows.

2 Governing Equations

For this paper, we restrict ourselves to isothermal constant density two-phase flow with no inter-phase mass transfer. Turbulence is modeled using the eddy viscosity hypothesis to close the Reynolds-averaged Navier-Stokes equations. The equations governing the hydrodynamics are:

**Momentum Equations**

\[
\frac{\partial}{\partial t} \left( \rho_\alpha r_\alpha U_\alpha^k \right) + \frac{\partial}{\partial x^i} \left( \rho_\alpha r_\alpha U_\alpha^i U_\alpha^k - r_\alpha \tau_\alpha^{ik} \right) = \rho_\alpha r_\alpha g^k - r_\alpha \frac{\partial P}{\partial x^k} + M_\alpha^k, \quad \alpha = 1,2
\]

**Continuity Equations**

\[
\frac{\partial}{\partial t} (\rho_\alpha r_\alpha) + \text{div}(\rho_\alpha r_\alpha U_\alpha) = 0, \quad \alpha = 1,2.
\]

**Total Volume Conservation Equation**

\[
\sum_\alpha r_\alpha = 1.
\]

Greek indices \(\alpha, \beta\) etc. are used to represent phases, and roman indices \(i, j, k\) etc. are used to denote vector and tensor components. For a given phase \(\alpha\), \(\rho_\alpha\) is the material density, \(r_\alpha\) is the volume fraction, and \(U_\alpha\) is the velocity. \(\tau_\alpha\) is the viscous stress tensor, with contributions from both molecular and eddy viscosity. The shared pressure assumption, \(P_\alpha = P\), is used for all phases.
\( M_\alpha \) are the interfacial forces between phases. They are assumed to take the form of simple isotropic inter-phase drag forces.

\[
M_\alpha = \sum_{\beta=1}^{N} c_{\alpha\beta} \left( U_\beta - U_\alpha \right), \quad c_{\alpha\beta} = c_{\beta\alpha} \geq 0. \tag{4}
\]

In 3 dimensions, eqns (1), (2), (3) form a closed system of 9 equations in 9 unknowns \( U_1, U_2, r_1, r_2, P \). Equations (1), (2) clearly take the form of transport equations for velocities and volume fractions, respectively. Moreover, under the assumption of constant density, eqns (2) and (3) together imply the \textit{flux conservation form} of the total volume conservation equation:

\[
\text{div} \left( \sum_{\alpha} r_\alpha U_\alpha \right) = 0. \tag{5}
\]

This is the correct analogue of the solenoidal velocity constraint in multi-phase flow and will be seen, in sections 3 and 4, to govern the pressure in the discretized equations.

In this work, eqns (1), (2), (3) are supplemented by a simple turbulence model which consists of:

- The standard \( k-\varepsilon \) model in the continuous phase, with volume fractions multiplying all flux and source terms.
- An algebraic eddy viscosity turbulence model in the dispersed phase, with the dispersed phase kinematic eddy viscosity assumed equal to that of the continuous phase:

\[
\nu_{td} = \nu_{tc} \Rightarrow \mu_{td} = \frac{\rho_d}{\rho_c} \mu_{tc}. \tag{6}
\]

3 Discretization

Spatial discretization is performed using the control volume, finite element method.

![Sub-control Volume](image)
Solution variables are co-located at element vertices, and control volumes are constructed as unions of element sub-control volumes, as illustrated in Figure 1 for quadratic elements.

Equations (1), (2), (3) are discretized by integrating over control volumes. By analogy with the single-phase case, terms linear in velocity and pressure are treated implicitly in both the momentum and continuity equations. All other terms are linearized with frozen coefficients.

**Momentum Equations**

\[
\frac{\rho_{\alpha\bar{r}}}{\delta t} V_i \left( \left( U_k^l \right)^{n+1}_i - \left( U_k^l \right)^n_i \right) + \left( A_{\alpha}^k \right)_j \left( U_k^l \right)^{n+1}_j = V_i \rho_{\alpha\bar{r}} g^k - \left( U_{\alpha,i}^l \right)^{n+1}_i + V_i \sum_{j} \left( \left( U_{\alpha,j}^l \right)^{n+1}_j - \left( U_{\alpha,i}^l \right)^{n+1}_i \right). \quad (7)
\]

**Continuity Equations**

\[
\frac{\rho_{\alpha\bar{r}} V_i}{\delta t} \left( r_{\alpha,i}^{n+1} - r_{\alpha,i}^n \right) + \sum_{i} \rho_{\alpha\bar{r}} \left( U_{\alpha,i}^l \cdot A_{i}^l \right)^{n+1}_i = 0. \quad (8)
\]

**Total Volume Conservation Equation**

\[
\sum_{\alpha} \sum_{i} r_{\alpha,i}^n \left( U_{\alpha,i}^l \cdot A_{i}^l \right)^{n+1}_i = 0. \quad (9)
\]

Superscripts \(n\) and \(n+1\) denote time levels, and \(k\) denotes Cartesian vector components. Subscripts \(i, j\), denote mesh vertices, and \(ip, jp\) denote integration points. \(\sum_{ip~i}\) denotes the sum over integration points adjacent to mesh vertex \(i\).

\(A_{ip}\) is the normal area vector of the control cell surface at \(ip\). \(A_{\alpha}^k\) denotes the advection-diffusion matrix for velocity component \(U_{\alpha}^k\). It is essential to use a positive advective interpolation scheme to obtain volume fractions at integration points. First order upwinding is used in this work.

Final closure of eqns (7), (8), (9) requires us to relate integration point velocities to mesh vertex fields. This is done using Rhie-Chow interpolation [3].
Computational Methods in Multiphase Flow

\[
(U_\alpha - \bar{U}_\alpha)_{ip}^{n+1} = d_{\alpha,ip}^n (\nabla P - \bar{\nabla} P)_{ip}^{n+1} + \frac{\rho_\alpha}{\delta t} d_{\alpha,ip}^n (U_\alpha^n - \bar{U}_\alpha^n)_{ip}
\]

(10)

\[d_{\alpha,ip}^n = \frac{r_{\alpha,ip}^n V_e}{A_{\alpha,ip}^n}\]

\(A_{\alpha,ip}\) is an approximation to the momentum equation matrix diagonal at integration points.

4 Solution Strategy

Substitution of eqn (10) into (7), (8), (9) results in a coupled 9x9 block linear system for the 9 variables \(U_1, U_2, r_1, r_2, P\) defined at mesh vertices.

\[
A^n \Phi^{n+1} = b^n \quad \Phi = (U_1, U_2, P, r_1, r_2).
\]

(11)

The sparse structure of the block matrix \(A\) is illustrated in Figure 2: Matrix rows are labeled by equation components, and columns are labeled by variable components. An empty block indicated a zero matrix.

\[
\begin{bmatrix}
U_1 & V_1 & W_1 & U_2 & V_2 & W_2 & P & r_1 & r_2 \\
\end{bmatrix}
\]

* = nearest neighbor coupled sparse matrix
\n = diagonally sparse matrix (point coupling only).

Figure 2: Block Sparse Matrix Structure for 2-Phase Hydrodynamics.

It can be seen, by inspection, that pressure is governed by the conservation of total volume equation, and that the frozen coefficient linearization of volume fractions in the continuity equations effectively de-couples the volume fractions.
from the block linear system. It is only necessary to solve the 7x7 subsystem for \((U_1, U_2, P)\). Volume fractions may be obtained subsequently by back substitution into the continuity equations.

On its own, such a strategy would require a CFL restriction on time step in the continuity equations both for stability and boundedness of the volume fractions. This is because eqn (8) is linearized explicitly with respect to volume fraction. This problem is avoided by replacing the explicit volume fraction update by a solution of the continuity eqns (2) discretized implicitly with respect to both velocity and volume fraction:

\[
\frac{\rho \alpha V_i}{\partial t} \left( r_{\alpha i}^{n+1} - r_{\alpha i}^n \right) + \sum_{ip} \rho \alpha r_{\alpha,ip}^{n+1} U_{\alpha,ip}^{n+1} \cdot A_{ip} = 0. \tag{12}
\]

The integration point velocities in eqn (12) are obtained from the solution of the 7x7 hydrodynamic sub-system. Unconverged solutions to eqn (12) do not necessarily satisfy the sum to unity constraint, eqn (3). Hence, the volume fractions are subsequently normalized:

\[
\hat{r}_{\alpha} = \frac{r_{\alpha}}{\sum_{\beta} r_{\beta}}. \tag{13}
\]

These normalized volume fractions are used in the linearization of equations at the next time step, and the process is repeated until convergence is obtained.

5 Airlift Loop Reactor Simulation

Becker, Sokolichin and Eigenberger [6] have studied several configurations of flat bubble columns with essentially a two-dimensional flow structure. The last case in their paper represents an airlift loop with non-trivial flow profiles but with sufficient geometrical restraint that the bubble column is least likely to be unsteady. This case is simulated for the purpose of evaluating the new multiphase solver.

5.1 Model

Figure 3 shows the geometry as well as the water flow and bubble distribution from a coarse grid solution obtained using the new CFX-5 multiphase solver. The computational domain covers the water-filled part of the column to a height of 1.75m. The width and thickness of the domain are 0.5 and 0.08 meters, respectively. Experimental velocity profile data are available at measuring stations at 300, 650, 1250 and 1650 mm above the floor. Air is injected asymmetrically through a frit sparger producing bubbles of order 3 mm diameter. The superficial gas velocity is 1.5cm/sec.
The air bubbles are modeled as the dispersed phase and water is modeled as the continuous phase. The bubbles experience a buoyancy force and a drag force based on the Grace correlation [7]. As described in section 2, the k-epsilon turbulence model is used in the continuous phase and an algebraic eddy viscosity is used in the dispersed phase.

The free surface is treated as a ‘degassing’ boundary condition, which the dispersed phase sees as an outlet and the continuous phase sees as a stress-free wall that prevents outflow. The liquid surface shape is assumed to be flat. Pressure is not prescribed, and any pressure variations computed at this surface represent the weight of local height variations in an actual free surface.

### 5.2 Computational grid

A two-dimensional hexahedral element grid is appropriate for an initial simulation of this geometry. In two dimensions, the inlet is represented as a slit of similar area and exact flow rate to the frit disc; in three dimensions, it is represented as a square.
Three levels of grid resolution are used to check grid dependence and computing effort. These length scales are based on using 10, 20 or 40 grid cells across the riser. The cells have a height to width ratio of order 1:1 in the cross flow regions at the top and bottom of the domain. But this ratio is increased to 9:1 to traverse the mid level of the column, where flow direction is mainly vertical.

Two-dimensional grids are used for direct comparison of the unstructured grid code CFX-5 with the block-structured hexahedral element code CFX-4. Some preliminary calculations were also performed on three-dimensional grids using CFX-5 only. For details, see Table 1.

5.3 Convergence

A trivial algebraic function is set to provide a plausible initial direction and velocity scale to the flow, as well as a degassing path. This case converges within 30-90 iterations in CFX-5 using an automatically computed time scale.

There is one corner at the highest point of the lower cross leg where bubbles can be trapped by the down flow. This one point appears to set a lower limit on the residuals achievable in a steady state simulation. The distribution of residuals indicates that solution elsewhere is well converged.

5.4 Validation

Figure 4 shows measured velocity profiles across the riser and those computed on the finest two-dimensional grid. The results for the medium resolution grid are similar.

Typically the vertical velocity of the bubbles is of order 0.2 m/sec over that of the water, since the bubbles quickly reach terminal velocity.

The agreement between CFD and experiment appears to be fair away from the inlet region. But other features of the flow are not predicted correctly: velocities close to the inlet region are over predicted; the vertical extent of a re-circulation at the right hand side of the riser (indicated in Figure 4 by a negative liquid velocity) is under predicted. The flow and bubble distribution is developing and non-homogeneous particularly in the inlet region. Also, there is a number of multi-phase modeling issues to be investigated further. Preliminary calculations suggest that three-dimensional effects and the modeling of a lift force term can each have a significant effect on the results.

Although there are minor differences in multi-phase turbulence modeling between CFX-4 and CFX-5, the good agreement between the codes provides additional validation of the new multiphase solver and of the basic multiphase physics implementation in CFX-5.
Figure 4: Comparison of Velocity Profiles.
5.5 Performance

Table 1: Performance of CFX-5 and CFX-4 on Various Grids.

<table>
<thead>
<tr>
<th>RESOLUTION</th>
<th>NODES</th>
<th>ITERATIONS</th>
<th>Effective CPU sec.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>CFX-4</td>
<td>CFX-5</td>
</tr>
<tr>
<td>2d-coarse</td>
<td>2068</td>
<td>187</td>
<td>42</td>
</tr>
<tr>
<td>2d-medium</td>
<td>7602</td>
<td>337</td>
<td>33</td>
</tr>
<tr>
<td>2d-fine</td>
<td>29930</td>
<td>982</td>
<td>40</td>
</tr>
<tr>
<td>3d-medium</td>
<td>41811</td>
<td>-</td>
<td>90</td>
</tr>
<tr>
<td>3d-fine</td>
<td>305655</td>
<td>-</td>
<td>55</td>
</tr>
</tbody>
</table>

*The data in this table is for a 466 MHz Digital AlphaServer 4100.

Table 1 compares the number of iterations and computing times for the new solver in CFX-5 and the segregated solver in CFX-4. These values were obtained by noting the iteration number and estimating the effective CPU time when the value of air volume fraction at a monitoring point on the degassing boundary is within 10% of its final value in a long run. This allows a grid and code independent comparison.

The first point to note in Table 1 is that the number of iterations needed for convergence is much less grid dependent in CFX-5 than in CFX-4. The second is that although the two-dimensional grids in this test are relatively small, the CFX-5 solution on the fine grid is already faster than the CFX-4 solution.

Table 2 shows the performance of CFX-5 in parallel computations. The test is performed using the three-dimensional medium resolution grid of 41811 vertices, and specifying a non-dimensional convergence criterion of $10^{-3}$. In this table, efficiency is defined as

$$\text{Efficiency} = \frac{\text{CPU time for serial run}}{100\% \times \text{Number of Processors} \times \text{Wall Clock Time}}$$

so that the contribution of communication time between processors is included.

Table 2: Performance of CFX-5 in Parallel.

<table>
<thead>
<tr>
<th>Processors</th>
<th>CPU seconds</th>
<th>Wall Clock seconds</th>
<th>Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1293</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>681</td>
<td>95%</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>500</td>
<td>86%</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>425</td>
<td>76%</td>
<td></td>
</tr>
</tbody>
</table>

*The data in this table is for a 667 MHz Digital (Compaq) AlphaServer ES40.

This three-dimensional multiphase problem is still not very large by industrial standards, but nevertheless is showing worthwhile reductions in clock time by using up to four processors.
6 Conclusions

In this paper we have demonstrated that the coupled solver technology employed in CFX-5 has been extended successfully to cover multiphase flow applications. For the validation problem presented in this paper, the solutions obtained from the coupled solver in CFX-5 and the segregated solver in CFX-4 are essentially the same, and close to the experimental values at least away from the inlet region. This comparison indicates that the new coupled solver solves the two phase equations correctly and captures the basics of bubbly flow physics.

The performance tests show that the good convergence characteristic, the linear scalability and good parallel performance of the coupled solver found in single phase flow applications hold true in the two phase flow application as well. The new solver in CFX-5 is proving to be an effective modeling tool for multi-phase flow simulation as models with large number of computational cells (order of millions) are becoming the norm.

References


