APPLICATION OF CFD TO MULTI-PHASE MIXING

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There have been significant developments in the application of Computational Fluid Dynamics (CFD) to problems in multi-phase mixing, through the application of 'Coupled Solvers', unstructured meshes and adaptive meshes. The paper summarises some of these developments in the CFX-5 software, and illustrates them on practical cases, including bubble columns and particle suspensions in mixing vessels, for which detailed validation is available.

CFD, CFX, Mixing, Multi-Phase Flows.

INTRODUCTION

There have been significant developments in the application of Computational Fluid Dynamics (CFD) to mixing-related problems through the application of 'Coupled Solvers', and developments in meshing, for example, unstructured meshes, Generalised Grid Interfaces and adaptive meshes. These developments are enabling much faster and reliable solutions for these problems, particularly in single-phase flows. More recently, these powerful techniques have become available for multi-phase flows, and they have the potential to improve significantly the prediction capabilities for mixing applications. This paper summarises some of these developments, and illustrates them on practical cases relevant to mixing problems.

SOLVER DEVELOPMENTS

COUPLED SOLVERS: CFX-5

Many CFD software packages are based around the use of 'segregated solvers', which solve the underlying conservation equations of Mass, Momentum and Energy, in a sequential fashion, using a 'pressure-correction' method. That is, with a guessed pressure field, the three momentum equations are solved one by one, for each of the velocity components, and then the pressure is calculated from the mass conservation equation, through a procedure such as the 'SIMPLE' algorithm. This inherently leads to many iterations being used to solve the non-linear system of equations, and requires expert knowledge of the convergence parameters.

With the 'coupled solver' approach, four linearised equations for Momentum and Mass conservation are solved simultaneously, without having to correct the pressure to give mass conservation. This approach reduces significantly the number of iterations required to obtain convergence, over the segregated approach, but it does require the solution of a large coupled system of linear equations. The key to the success of the approach is a fast 'Algebraic Multi-Grid' (AMG) solution technique, for the solution of the coupled system of linear equations, Raw[2]. This allows the solution to be solved in far fewer iterations than for pressure-correction methods, and the success of the approach has been demonstrated on many single-phase flows, ranging from non-Newtonian, through to high Mach Number flows. The coupled solver method is implemented in the CFX-5 software, along with a general unstructured mesh, consisting of tetrahedral, hexahedral, prismatic and wedge elements. This software, coupled to semi-automatic mesh generation, gives much faster set up and solution times.

MULTI-FLUID MODELS

Multi-Phase flow models are conventionally represented using a Multi-Fluid approach, where each phase is represented as a separate fluid, each with its own velocity field, and a common pressure field. An extension of the pressure correction schemes, such as the IPSA algorithm, can be used to calculate the volume fractions and the common pressure. Most software packages use a simplification of the general method, using only two fluids, to give the Two-Fluid Model, with one velocity field representing a continuous phase, and another a dispersed phase. It can be extended to more than two fluids, but convergence of the resulting equations can be difficult to obtain with segregated solvers. It has also been extended to include the prediction of bubble sizes, through the use of a population balance model, such as the MUSIG model implemented in the CFX-4 software. This approach has now led to an number of industrial success stories, although major limiting factors are the computing requirements for these models, and the convergence issues, especially for finer grids, using segregated solvers.

Recently, the coupled-solver approach described above for CFX-5, has been extended from single-phase flows, to multi-phase flows, see for example, Yin, et al[1]., with the AMG method extended to handle the larger system of linear equations resulting from the use of the Multi-Fluid method. This offers significant potential for the solution of mixing problems, where one of the main bottlenecks is the computing time required to get solutions to Engineering problems, in a complex geometry, with realistic physical models for the flow. The basis for this is described in detail in Yin, Burns, Splawski and Guetari[1], and is available in CFX 5.5.

GENERALISED GRID INTERFACES

For mixing vessels and other systems comprising rotating and stationary components, it is convenient to solve the system using two grid systems, one rotating with the impeller, and one static around the periphery of the mixing vessel and baffles. This results in meshes that are discontinuous at the interface of these two regions, where a ‘Generalised Grid Interface’ is required to transfer the information from one region to another, where the mesh points are not coincident. The same approach can also be used to embed a fine grid within a coarser grid, in order to resolve fine details of the flow. At this interface, it is necessary to be able to maintain the accuracy of the discretisation, and also mass conservation. This is especially important in a multi-phase flow, where there are mass conservation equations for each phase. This approach in CFX-5.5.1 ensures this takes place. The flow in such cases is inherently transient, and therefore computationally very expensive if solved in a transient fasion. There are, however, two simplifications that can give rise to quasi-steady state solutions through the averaged procedure, where the flows are averaged circumferentially, or through a frozen rotor approximation where the impeller is fixed at a particular angle.

RESULTS

Many different test cases have been studied using CFX 5.5.1, for bubbly flows and particle-laden flows, both of which are relevant in mixing processes, for example in catalytic processes. The results presented here show the benefits from the methods for simple problems for which comparison information is available. These include:

- Bubble Columns
- Predictions of Bubble Size Distributions using a Population Balance Model.
- Use of a Four fluid model for a problem with a particle size distribution
- Demonstration of the multi-fluid model in a Mixing Vessel

BUBBLE COLUMN

The first case to be looked at is a bubble column, for which detailed experimental results are available, along with results from CFX-4 which has been extensively validated for bubbly flows. The bubble column studied is shown in Figure 1.

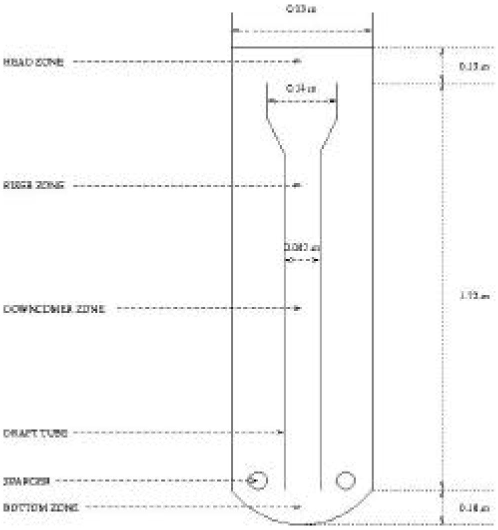

Figure1: Sketch of the Bubble Column Reactor

Figure 2 shows a comparison between the CFX-5.5 results for the Gas holdup against superficial gas velocity, using a hexahedral and tetrahedral grid, the experimental results of Pfleger and Becker[4], and results from CFX-4 calculations. For CFX-5, solver convergence was generally achieved between 60 and 100 iterations. For a segregated solver, many more coefficient loops are required for this kind of application.

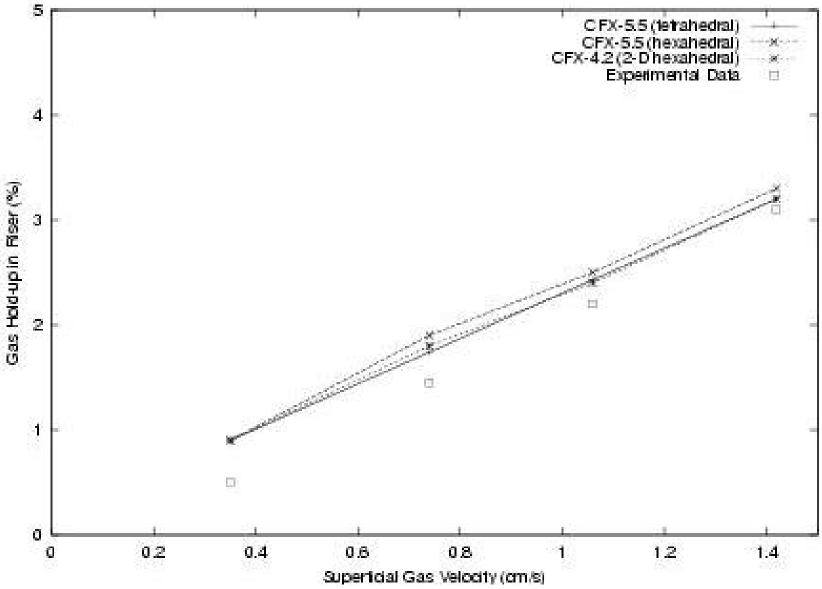

Figure2: Gas holdup vs Superficial Velocity

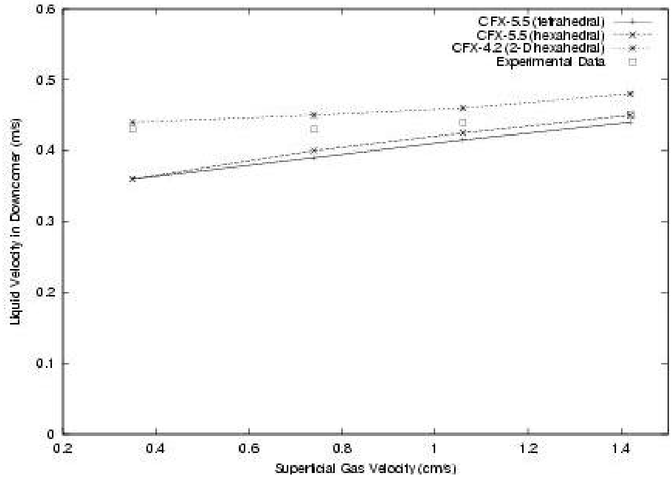

Figure 3: Liquid Flow Rate in the Downcomer; Predictions and Experimental Values.

Figure 3 shows the predictions for the liquid flow rate at one location in the downcomer, compared to the results for CFX-4 and experiments. The agreement with experiment is good, especially for hexahedral elements in CFX-5.

The parallel efficiency of the Coupled Solver implementation is generally good, and is illustrated in Fig 4 below, showing good speed-ups for this case on both a Linux cluster, and an SGI Unix system.

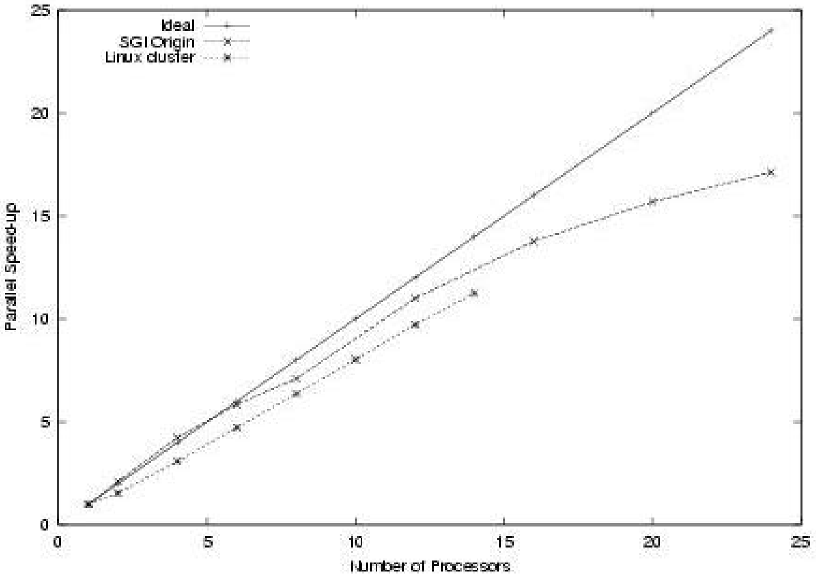

Figure 4: Parallel Speed Ups for the Bubble Column Reactor, Unix and Linux Systems.

More detailed results for this case are given in Zwart et al,[4]

Further calculations for a simplified Bubble Column have been carried out using a population balance model, the MUSIG model, to predict the distribution of bubble sizes, and also the interfacial area density, an important quantity for mass transfer. The figures below in Figure 5 show the predicted values for this in the column. These are in broad agreement with the earlier CFX-4 results for this configuration, Montavon and Hamill [5]

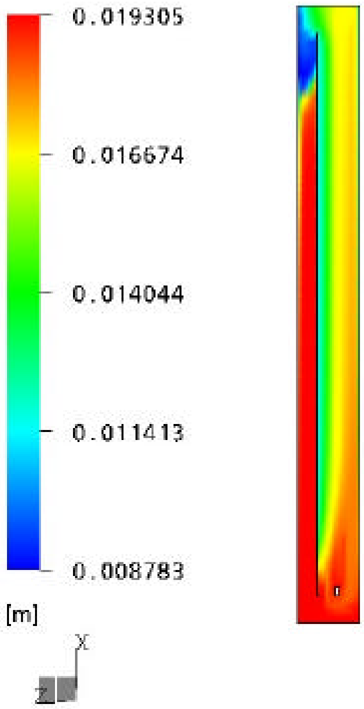

Figure 5a: Sauter Mean Diameter

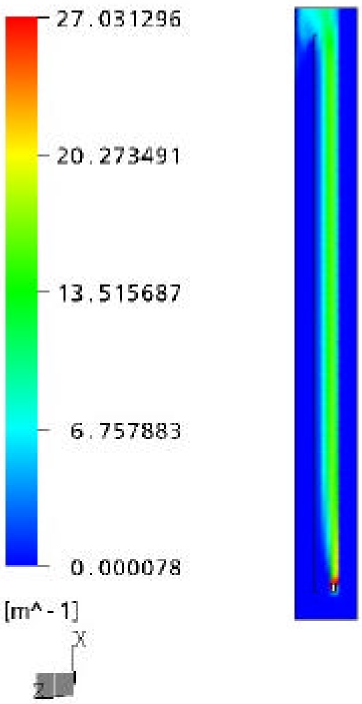

Figure 5b: Interfacial Area Density

FOUR-FLUID MODELS

The above calculations have been carried out using a two-fluid model, with only two velocity fields. As a demonstration of the capability of the coupled solver approach, detailed calculations have been carried out for a device where particles of three different sizes, 20, 500 and 1500 microns are injected, and it is required to know the resulting solids distribution.

These calculations were run on a Dell PC with twin 1.7 GHz processors and Linux O/S . The single–phase results took around 100 iterations in 30 mins and used 80 Mb RAM. The corresponding Eulerian four-phase simulations only required 135 iterations, and took 4.6 hours. This demonstrates only a small degredation in performance due to the use of several fluids in a Multi-Fluid model. This method therefore has great potential for other simulations where there may be a particle size distribution.

MIXING VESSEL

The next example chosen is a multi-impeller reactor with 4 pitched blade impellers, with a solid suspension, for which experimental results and simulations from CFX-4 are available, Montante et al[6]

These calculations were carried out using the Generalized Grid Interface around each of the impellers, with a 'frozen rotor'. This enabled the calcuation to be solved as a steady state simulation. Details of the numerical approach are presented in Svihla and Guetari[7].

Figure 6a shows the configuration for this case, along with streamlines illustrating the complex flow patterns in the configuration, and Figure 6b, the dimensionless solids concentrations. These are consistent with the results of Montante et al [6]. More detailed comparisons with these experiments are currently being carried out.

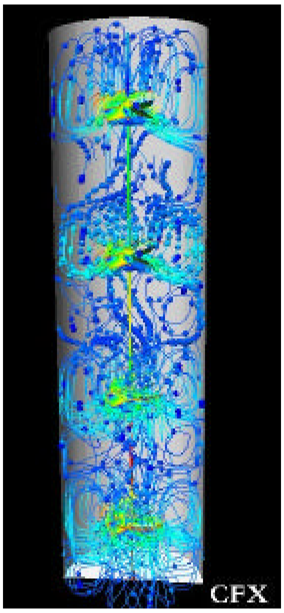

Figure 6a: Streamlines in the mixing tank

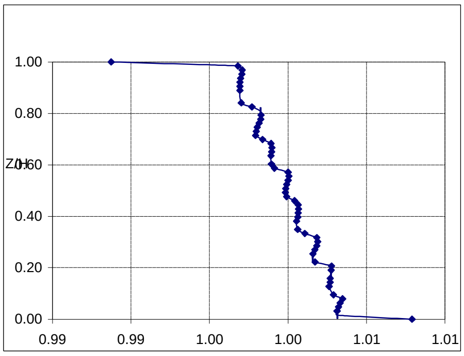

Figure 6b: Dimensionless Solids Concentration as a function of height.

CONCLUDING REMARKS

This paper has presented some results to demonstrate the progress that has been made in the modelling of complex multi-phase flows. In particular, the use of coupled solvers for the Multi-Phase flows, together with features such as the Population Balance Models and Generalised Grid Interfaces, is enabling the incorporation of more realistic physical models, much more quickly than in previous generations of CFD software.

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