ON THE PERFORMANCE OF MASS CONSERVATION BASED ALGORITHMS FOR MULTI-PHASE FLOWS

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ABSTRACT

This work is concerned with the implementation and testing, of four incompressible-segregated multi-phase flow algorithms that belong to the Mass Conservation Based Algorithms (MCBA) group in which the pressure correction equation is derived from overall mass conservation. The pressure correction schemes in these algorithms are based on SIMPLE, SIMPLEX, PISO, and PRIME. Solving two one-dimensional two-phase flow problems spanning the spectrum from bubbly to gas-solid flows assesses the performance and accuracy of the multi-phase algorithms. The main outcome of this study is a clear demonstration of the capability of all MCBA algorithms to deal with multi-phase flow situations. Moreover, results displayed in terms of convergence history plots and CPU-times, indicate that the performances of the MCBA versions of SIMPLE and SIMPLEX are very close. As expected, the PRIME algorithm is found to be the most expensive due to its explicit treatment of the phasic momentum equations. The PISO algorithm is generally more expensive than SIMPLE and its performance depends on the type of flow and solution method used.

KEY WORDS

Multi-phase algorithms, bubbly flows, air-particle flows.

1. INTRODUCTION

The extensive developments that have taken place in Computational Fluid Dynamics (CFD) over the last three decades have established this still evolving technology as a reliable and essential tool for the simulation and optimization of a wide variety of engineering fluid flow processes (mixing, solidification, turbulence, …). Several issues that were hindering its progress have been addressed and remedies suggested. Concerns related to accuracy were assuaged through the development of High Resolution (HR) schemes [1-3]. Moreover, better solution algorithms [4-7], solvers, and multi-grid techniques have greatly reduced the computational cost and made it feasible to solve real life problems.

While high-resolution schemes, solvers, multi-grid techniques, etc… can be applied to simulate both single- and multi-phase flows, nearly all developments in solution algorithms have been directed towards the simulation of single-fluid flow. In particular, many segregated single-fluid solution algorithms were developed such as the well-known SIMPLE [4], PISO [5], PRIME [8], and SIMPLEX [6] algorithms, to site a few.

On the other hand, developments in solution algorithms for simulating multi-phase flow phenomena have lagged behind that of single-phase flow algorithms due to the much higher computational cost involved, the numerical difficulties that had to be first addressed in the simulation of single-phase flow, and the increase in algorithmic complexity. While the major difficulties in the simulation of single-phase flow stems from the coupling between the momentum and continuity equations, in the simulation of multi-phase flow phenomena, this problem is further complicated by the fact that there are as many sets of continuity and momentum equations as there are fluids, that they are all coupled together in various ways and that the fluids share space.

Despite these complexities, successful segregated pressure-based solution algorithms have been devised. The IPSA variants devised by the Spalding group at Imperial College [9] and the set of algorithms devised by the Los Alamos Scientific Laboratory (LASL) group [10] are examples of multi-phase algorithms.

Recently, Darwish et al. [11] extended the large number of segregated single-fluid flow algorithms reviewed in [7] to predict multi-phase flow phenomena and showed that the pressure correction equation can be derived either by using the geometric conservation equation or the overall mass conservation equation. Depending on the chosen equation, the segregated pressure-based multi-phase flow algorithms were classified as either the Geometric Conservation Based family of Algorithms (GCBA) or the Mass Conservation Based family of Algorithms (MCBA). Many of these algorithms have neither been tested nor implemented in CFD codes.

The objective of the present work is to implement and test four multi-phase algorithms from the MCBA group and to assess their relative performance by solving two one-dimensional incompressible two-phase flow problems encompassing gas-solid flows in addition to bubbly flows on several grid sizes.

2. THE GOVERNING EQUATIONS

In incompressible multi-phase flow the various fluids/phases coexist with different concentrations at different locations in the flow domain and move with unequal velocities. Thus, the equations governing multi-phase flows are the conservation laws of mass and momentum for each individual fluid.

If a typical representative variable associated with phase (k) is denoted by $\phi^{k)}$, the conservation equations can be written using a general phasic equation as:

$$\frac{\partial}{\partial t}\left(r^{(k)}\rho^{(k)}\phi^{(k)}\right)+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}\right)= \nabla.\left(r^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}\right)+r^{(k)}Q^{(k)} \tag{1}$$

where $r^{(k)}$ refers to the volume fraction ($\Omega^{(k)}/\Omega$), $\rho^{(k)}$ the phasic density, and $u^{(k)}$ the velocity vector. Moreover, the diffusion coefficient $\Gamma^{(k)}$ and source term $Q^{(k)}$ are specific for a particular meaning of ϕ.

For incompressible laminar multi-phase flow, auxiliary relations are needed to close the system of equations including the geometric conservation equation $\sum r^{(k)}=1$ and the interfacial mass and momentum transfers. In this work, only interfacial momentum transfer is of interest and its closure will be detailed later.

2. DISCRETIZATION PROCEDURE

The general conservation equation (1) is integrated over a finite volumeto yield:

$$\iint_{\Omega}\frac{\partial\left(r^{(k)}\rho^{(k)}\phi^{(k)}\right)}{\partial t}d\Omega+\iint_{\Omega}\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}\right)d\Omega =\iint_{\Omega}\nabla.\left(r^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}\right)d\Omega+\iint_{\Omega}r^{(k)}Q^{(k)}d\Omega \tag{2}$$

Where Ω is the volume of the control cell. Using the divergence theorem to transform the volume integral into a surface integral, replacing the surface integrals by a summation of the fluxes over the sides of the control volume, and then discretizing these fluxes using suitable interpolation profiles (the High Resolution SMART [1] scheme is employed and applied within the context of the NVSF methodology [3]) the following algebraic equation results:

$$A_P^{(k)}\phi_P^{(k)}=\sum_{NB}A_{NB}^{(k)}\phi_{NB}^{(k)}+B_P^{(k)} \tag{3}$$

In compact form, the above equation can be written as

$$\phi^{(k)}=H_P\left[\phi^{(k)}\right]=\frac{\sum_{NB}A_{NB}^{(k)}\phi_{NB}^{(k)}+B_P^{(k)}}{A_P^{(k)}} \tag{4}$$

An equation similar to equation (4) is obtained at each grid point in the domain and the collection of these equations forms a system that is solved iteratively.

The discretization procedure for the momentum equation yields an algebraic equation of the form:

$$\mathbf{u}_P^{(k)}=\mathbf{HP}_P\left[\mathbf{u}^{(k)}\right]-r^{(k)}\mathbf{D}_P^{(k)}\nabla_P(P) \tag{5}$$

Furthermore, the phasic mass-conservation equation can be viewed as a phasic volume fraction equation, which can be written as:

$$r_P^{(k)}=H_P\left[r^{(k)}\right] \tag{6}$$

or as a phasic continuity equation to be used in deriving the pressure correction equation:

$$\frac{\left(r_P^{(k)}\rho_P^{(k)}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega+ \Delta_P\left[r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}.\mathbf{S}\right]=r^{(k)}\dot{M}^{(k)} \tag{7}$$

where the Δ operator represents the following operation:

$$\Delta_P\left[\Theta\right]=\sum_{f=nb(P)}\Theta_f \tag{8}$$

3. PRESSURE CORRECTION EQUATION

To derive the pressure-correction equation, the mass conservation equations of the various fluids are added to yield the global mass conservation equation given by:

$$\sum_k\left\{\frac{\left(r_P^{(k)}\rho_P^{(k)}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega+ \Delta_P\left(r^{(k)}\rho_P^{(k)}\mathbf{u}^{(k)}.\mathbf{S}\right)\right\}=0 \tag{9}$$

Denoting the corrections for pressure and velocity by P' and $\mathbf{u}^{(k)'}$, respectively, the corrected fields are written as:

$$P=P^{\circ}+P',\mathbf{u}^{(k)}=\mathbf{u}^{(k)^*}+\mathbf{u}^{(k)'} \tag{10}$$

Combining equations (5), (9), and (10), the final form of the pressure-correction equation is obtained as:

$$\sum_k\left\{\Delta_P\left[r^{(k)^{\circ}}\rho^{(k)*}\left(r^{(k)^{\circ}}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\}= \sum_k\left\{\begin{array}{l}\dfrac{r_P^{(k)\circ}\rho_P^{(k)*}-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega\\ +\Delta_P\left[r^{(k)\circ}\rho^{(k)*}U^{(k)*}\right]\\ +\Delta_P\left[r^{(k)^{\circ}}\rho^{(k)*}\left(\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]\right).\mathbf{S}\right]\end{array}\right\} \tag{11}$$

If the $\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]$ term in the above equation is retained, there will result a pressure correction equation relating the pressure correction value at a point to all values in the domain. To facilitate implementation and reduce cost, simplifying assumptions related to this term have been introduced. Depending on these assumptions, different algorithms are obtained. These algorithms were accorded a full-length paper [11] of discussion to which interested readers are referred. The corrections are then applied to the velocity and pressure fields using the following equations:

$$\mathbf{u}_P^{(k)*} = \mathbf{u}_P^{(k)\mathrm{o}} - r^{(k)\mathrm{o}} \mathbf{D}_P^{(k)} \nabla_P P', P^* = P^{\mathrm{o}} + P' \quad (12)$$

4. THE MCBA SOLUTION PROCEDURE

The sequence of events in the MCBA is as follows:

Solve the phasic momentum equations for velocities.

Solve the pressure correction equation based on global mass conservation.

Correct velocities and pressure.

Solve the phasic mass conservation equations for volume fractions.

Return to the first step and repeat until convergence.

5. RESULTS AND DISCUSSION

Due to the large number of parameters affecting the performance of the various multi-phase Mass Conservation Based Algorithms and to allow a thorough testing of these algorithms, one-dimensional two-phase flow problems are considered. A total of eight problems have been thoroughly investigated ranging from dilute bubbly flows to dense gas-solid flows. Due to space limitation only two representative problems are discussed here. The first one deals with a gas-solid situation whereas the second problem is concerned with a bubbly flow. Results are presented in terms of the convergence history and the CPU-time needed to converge the solution to a set level. Predictions are compared against available numerical/theoretical values.

Computations are terminated when the maximum normalized residual of all variables drops below a very small number ε_s. In general, it is found that requiring the overall mass residuals to be satisfied to within ε_s is a very stringent and sufficient requirement. The effects of grid refinement on accuracy and convergence are studied by solving the problems on four grid systems of sizes 20, 40, 80, and 160 control volumes with ε_s assigned the value of 10^{-8}.

To allow a comparative assessment of performance, the CPU times are reported in the form of charts. Moreover, all CPU times are normalized by the time needed by MCBA-SIMPLE to reach the set residuals on the coarsest grid.

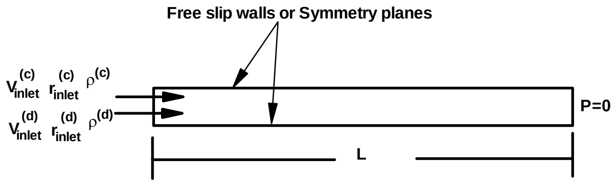


Fig. 1 Physical domain.

Problem 1: Gas-solid flow

The physical situation is depicted in Fig. 1. Depending on the set densities, it represents either the steady flow of solid particles suspended in a free stream of air or the steady flow of air bubbles in a stream of water. The slip between the phases determines the drag, which is the sole driving force for the particle-bubble/air-water motion (g=0). In the suspension, the inter-particle/bubble forces are neglected. Diffusion within both phases is set to zero while the inter-phase drag force is calculated as:

$$I_M^{(c)} = -I_M^{(d)} = \frac{3}{8}\frac{C_D}{r_p} r^{(d)} \rho^{(c)} V_{slip} \left(u^{(d)} - u^{(c)}\right) \quad (13)$$

$$V_{slip} = \left\| \mathbf{u}^{(d)} - \mathbf{u}^{(c)} \right\| \quad (14)$$

The drag coefficient, C_D, is set to 0.44. The task is to calculate the particle/bubble-velocity distribution as a function of position. If the flow field is extended far enough (here computations are performed over a length of L=2m), the particle/bubble and fluid phases are expected to approach an equilibrium velocity given by:

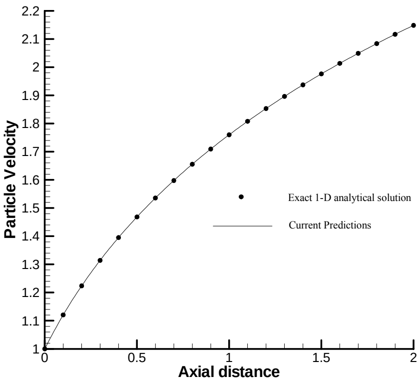
$$\mathrm{U}_{\mathrm{equilibrium}} = \mathrm{r}_{\mathrm{inlet}}^{(\mathrm{c})} \mathrm{V}_{\mathrm{inlet}}^{(\mathrm{c})} + \mathrm{r}_{\mathrm{inlet}}^{(\mathrm{d})} \mathrm{V}_{\mathrm{inlet}}^{(\mathrm{d})} \quad (15)$$

At inlet, the air and particle velocities are 5 m/s and 1 m/s, respectively. The physical properties of the two phases are: $\rho^{(d)} / \rho^{(c)} = 2000, r_p = 1\,mm, r_{inlet}^{(d)} = 10^{-5}$. Due to the dilute concentration of the particles, the free stream velocity is more or less unaffected by their presence and the equilibrium velocity is nearly equal to the inlet free stream velocity. Based on this observation, Morsi and Alexander [12] obtained an analytical solution for the particle velocity $u^{(d)}$ as a function of the position x.

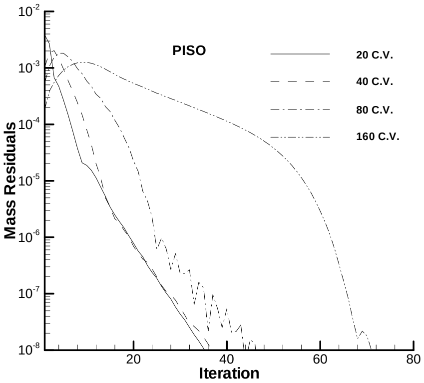
As shown in Fig. 2(a) the predicted particle velocity distribution falls on top of the analytical solution [12], which is an indication of the accuracy of the numerical procedure. The convergence histories of the various MCBA over the four grid networks used are displayed in Figs. 2(b)-2(e). For all algorithms, the required number of iterations increases as the grid size increases, with PISO (Fig. 2(b)) requiring the minimum and PRIME (Fig. 2(d)) the maximum number of iterations on all grids. The convergence histories of SIMPLE and SIMPLEX (Figs. 2(c) and 2(e), respectively) are very similar requiring nearly the same number of iterations on all grids.

Problem 2: Bubbly flow

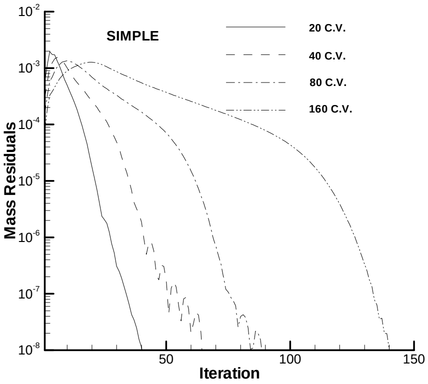
For the same configuration displayed in Fig. 1, the continuous phase is considered to be water and the disperse phase to be air. The resulting flow is denoted in the literature by bubbly flow. With the exception of $\rho^{(d)} / \rho^{(c)} = 10^{-3}$ and at inlet $r_{inlet}^{(d)} = 0.1$, other physical properties and inlet conditions are the same as those considered earlier. The correct physical solution is that the bubble and continuous phase velocities both reach the equilibrium velocity of 4.6 m/s (Eq. (15)) in a distance too small to be correctly resolved by any of the grid networks used. Results for this case are presented in Fig. 3. Axial velocity distribution for both water and air are displayed in Fig. 3(a). As expected, both phases reach the equilibrium velocity of 4.6 m/s over a very short distance from the inlet section and remain constant afterward. The relative convergence characteristics of the various algorithms remain the same. However, all algorithms require larger number of iterations as compared to the gas solid flow case due to the stronger coupling between the phases. Consistently, the PISO (Fig. 3(b)) and PRIME (Fig. 3(d)) algorithms need the lowest and highest number of iterations, respectively. As in the previous two cases, the convergence attributes of SIMPLE (Fig. 3(c)) and SIMPLEX (Fig. 3(e)) are very similar.



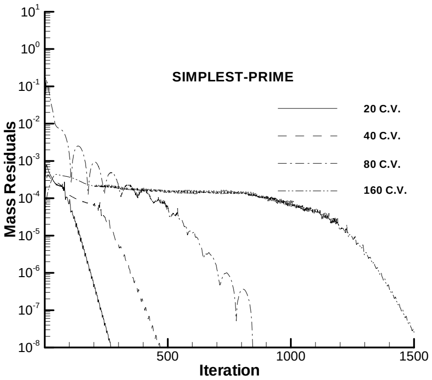
(a)



(b)



(c)



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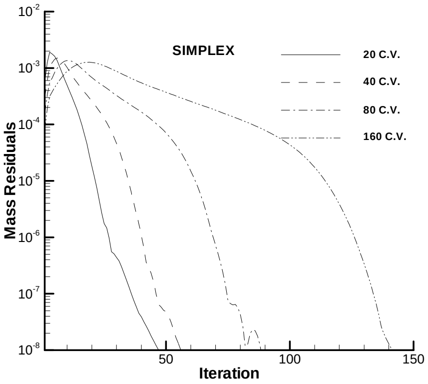


(e)

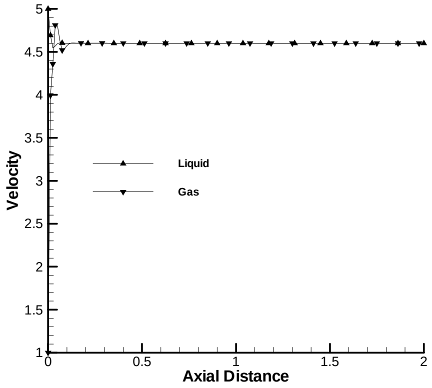
Fig. 2 (a) Comparison between the analytical and numerical particle velocity distributions, (b)-(e) convergence histories on the different grid systems.

CPU time

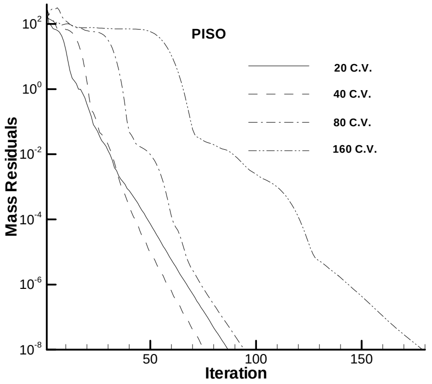
The normalized CPU efforts required by the various algorithms over all grids are depicted in Fig. 4. The charts clearly show that the CPU time increases with increasing grid density. For the gas-solid problem (Fig. 4(a)), it is hard to see any noticeable difference in the CPU times for SIMPLE, SIMPLEX, and PISO. The worst performance is for PRIME, which uses a fully explicit solution scheme.

The normalized CPU time of PRIME for the bubbly flow problem (Figs. 4(b)) is lower than in the previous problem due to a higher rate of increase in the time needed by other algorithms (the computational time of all algorithms has increased). The relative performance of the various algorithms is nearly as described earlier with the time required by of PISO, SIMPLE, and SIMPLEX being on average the same. The PRIME algorithm however, requires nearly three folds the time needed by SIMPLE, which represents a noticeable improvement.

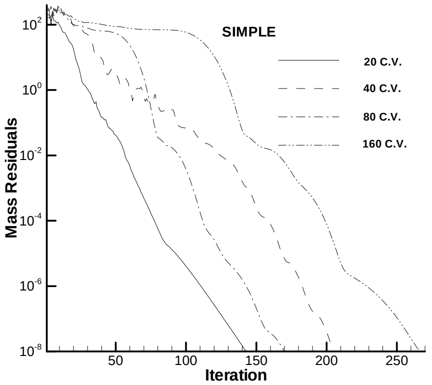
By comparing the behavior of the various algorithms in both problems, it is clear that the performance of SIMPLE and SIMPLEX is consistent and require, on average, the least computational effort. The PRIME algorithm is the most expensive to use on all grids and for all physical situations presented here. Most importantly however, is the fact that all these algorithms can be used to predict multi-phase (in this case two-phase) flows.



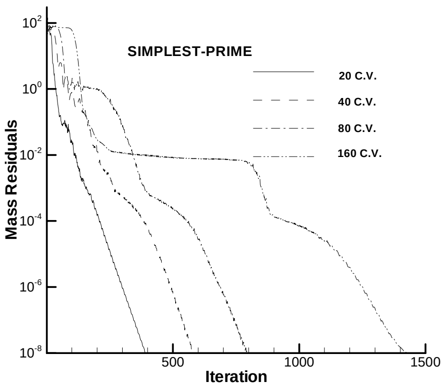
(a)



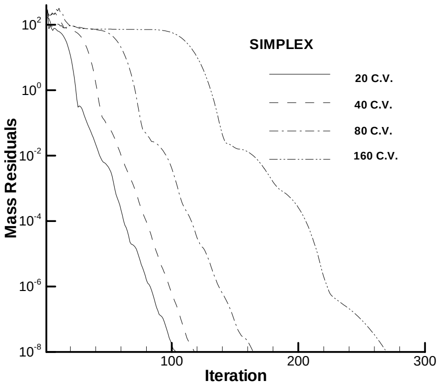
(b)



(c)

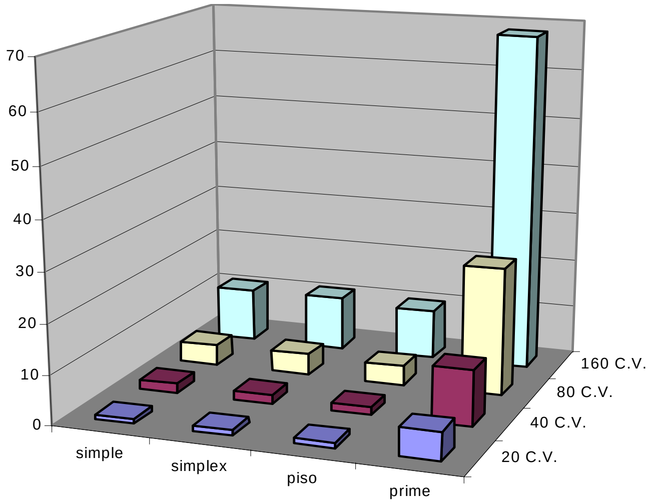


(d)

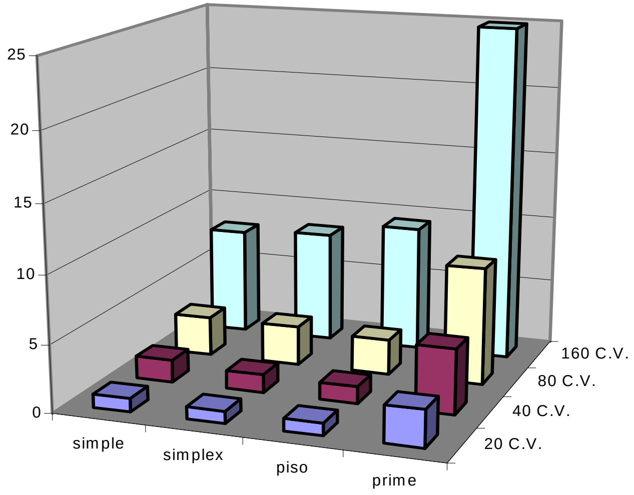


(e)

Fig. 3 (a) Liquid and gas velocity distributions, (b)-(e) convergence histories on the different grid systems.



(a)



(b)

Fig. 4 Normalized CPU-times for the horizontal (a) gas-solid, and (b) bubbly flow problem.

5. CONCLUSION

Four MCBA algorithms for the simulation of incompressible multi-phase flows were implemented, tested, and their relative performance assessed by solving a variety of one-dimensional two-phase flow problems. Results obtained demonstrated that all MCBA multi-phase algorithms are capable of dealing with a wide variety of incompressible multi-phase flow problems. The convergence history plots and CPU-times presented, indicated similar performances for SIMPLE and SIMPLEX. The PISO algorithm was in general more expensive than SIMPLE. Moreover, the PRIME algorithm was the most expensive to use.

6. ACKNOWLEDGEMENT

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REFERENCES

[1] Gaskell, P.H. and Lau, A.K.C., Curvature Compensated Convective Transport: SMART, A New Boundedness Preserving Transport Algorithm, *Int. J. Num. Meth. Fluids*, 8, 1988, 617-641.

[2] Leonard, B.P., Locally Modified Quick Scheme for Highly Convective 2-D and 3-D Flows, in Taylor, C. and Morgan, K. (Eds.) *Numerical Methods in Laminar and Turbulent Flows*, 15 (Swansea, U.K: Pineridge Press, 1987) 35-47.

[3] Darwish, M.S. and Moukalled, F., Normalized Variable and Space Formulation Methodology For High-Resolution Schemes, *Numerical Heat Transfer*, Part B, 26, 1994, 79-96.

[4] Patankar , S.V. and Spalding, D.B., A Calculation Procedure for Heat, Mass and Momentum Transfer in Three Dimensional Parabolic Flows, *Int. J. Heat & Mass Trans.*, 15, 1972, 1787-1806.

[5] Issa, R.I., Solution of the Implicit Discretized Fluid Flow Equations by Operator Splitting, Mechanical Engineering Report, FS/82/15, (Imperial College, London, 1982).

[6] Van Doormaal, J. P. and Raithby, G. D., An Evaluation of the Segregated Approach for Predicting Incompressible Fluid Flows, ASME Paper 85-HT-9, *Proc. National Heat Transfer Conference*, Denver, Colorado, August 4-7, 1985.

[7] Moukalled, F. and Darwish, M., A Unified Formulation of the Segregated Class of Algorithms for Fluid Flow at All Speeds, *Numerical Heat Transfer*, Part B, 40, 2001, 99-137.

[8] Maliska, C.R. and Raithby, G.D., Calculating 3-D fluid Flows Using non-orthogonal Grid, *Proc. Third Int. Conf. on Numerical Methods in Laminar and Turbulent Flows*, Seattle, 1983, 656-666.

[9] Spalding, D.B., Numerical Computation of Multi-Phase Fluid Flow and Heat Transfer, in Taylor C. and Morgan K. (Eds.), *Recent Advances in Numerical Methods in Fluid*, 1, 1980, 139-167.

[10] Amsden, A.A., Harlow F.H., KACHINA: An Eulerian Computer Program for Multifield Flows, Report LA-NUREG-5680, 1975.

[11] Darwish, M., Moukalled, F., and., Sekar, B., A Unified Formulation of the Segregated Class of Algorithms for Multi-phase Flow at All Speeds, *Numerical Heat Transfer*, Part B, 40(2), 2001, 99-137.

[12] Morsi, S.A. and Alexander, A.J., An investigation of Particle Trajectories in Two-Phase Flow System, *Journal of Fluid Mechanics*, 55(2),1972, 193-208.

[13] Baghdadi, A.H.A. *Numerical Modelling of Two-Phase Flow With Inter-Phase Slip*, Ph.D. Thesis, Imperial College, University of London, 1979.