Implementation of a Two-phase Three-field Model on an Unstructured-mesh Pressure-based Algorithm

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1. Introduction

Over the past three decades, many researches have been conducted in computational fluid dynamics (CFD). The main outputs from the researches are wide spread in numerics and physics, for example, developments of solution algorithms for the Navier-Stokes equations and numerical schemes for a high-resolution, and modeling of turbulence, combustion, and multi-phase. For the multi-phase flow analysis, many CFD algorithms have been implemented. The density-base or pressure-based preconditioned coupled algorithm was used in the OVAP code [1]. Theoretically, the fully coupled method is very stable and efficient computationally. But it is difficult to derive an upwind flux and to implement physical models for the multi-phase flows. Implicit-Continuous-Eulerian (ICE) algorithm, which was used in the RELAP and MARS codes, has been implemented into the 3-D multi-phase CFD code [2]. In the method, because the equations are coupled by a chain rule at each grid point, it is very stable for inter-phasic exchanges. But because of the decoupling between the computational nodes or cells, the computational time step is limited by convective and diffusive time scales. For many years, the projection method such as the fractional-step or SMAC method has been used for the multi-phase flow analysis. It is very efficient for the unsteady calculations by the nature of the non-iterative scheme. On the contrary because of the phasic decoupling, it is known that a phase change between liquid and vapor is difficult to resolve. The SIMPLEbased algorithms have been popularly used for the general fluid and heat transfer problems such as internal and external turbulent flows and species transport problems with or without combustion. In contrast to the above mentioned ICE and projection method, it is based on an iterative or multi-correction scheme in order to satisfy a mass conservation and to couple the variables in the equations. The time accuracy of a solution can be obtained by a marching in time, in addition to the multicorrection. Because the convective, diffusive and source terms are implicitly discretized, the computational time step is mostly defined based on a physical time step which must be resolved. Even though it has some limitations or weaknesses for the multi-phase flow analyses, some commercial CFD codes for the multiphase flows have been developed by extending the single-phase flow solvers which are based on SIMPLElike algorithm. The vendors of the commercial CFD codes are still under modification of the algorithm and development of physical models for the multi-phase flows.

In this study, a three-field two-phase CFD code based on the SIMPLE algorithm has been being developed in order to analyze two-phase thermo-hydraulic phenomena in a water-cooled nuclear power plant. The three fields include vapor, droplets, and continuous liquid. Their governing equations are time-spaceaveraged mass, momentum and energy equations for each field. It was assumed that the continuous liquid and droplets fields are in a thermally equilibrium state. In order to easily resolve the complex geometry encountered in modeling of the components of the plant such as a reactor vessel or a steam generator, a hybrid unstructured mesh technology was adopted, where hexahedral cells are generated globally and tetrahedral, prismatic and pyramid cells are locally embedded. The momentum equations are coupled among phases and solved with a sparse block Gauss-Seidel matrix solver in each Cartesian coordinate direction. The pressure correction equation is derived by summing the phasic volume fraction equations.

In this article, the numerical characteristics of the code are investigated for the analyses of basic two-phase flows.

2. Governing Equations

The governing equations of a three-field two-phase model describe the mass, momentum and energy conservations for each phase.

$$\frac{\partial}{\partial t} (\alpha_{k} \rho_{k}) + \nabla \cdot (\alpha_{k} \rho_{k} \overset{\mathbf{r}}{u_{k}}) = \Omega_{k}$$
(1)
$$\frac{\partial}{\partial t} (\alpha_{k} \rho_{k} \overset{\mathbf{r}}{u_{k}}) + \nabla \cdot (\alpha_{k} \rho_{k} \overset{\mathbf{r}}{u_{k}} \overset{\mathbf{r}}{u_{k}}) - \nabla \cdot (\alpha_{k} \mathbf{T}_{k})$$

$$= \alpha_{k} \rho_{k} \overset{\mathbf{r}}{g} - \alpha_{k} \nabla p + \mathbf{M}_{k}^{mass} + \mathbf{M}_{k}^{drag} + \mathbf{M}_{k}^{YM}$$

$$\frac{\partial (\alpha_{k} \rho_{k} e_{k})}{\partial t} + \nabla \cdot (\alpha_{k} \rho_{k} e_{k} \overset{\mathbf{r}}{u_{k}}) - \nabla \cdot (\alpha_{k} \overset{\mathbf{r}}{q}_{k})$$

$$= \alpha_{k} \mathbf{T}_{k} : \nabla \overset{\mathbf{r}}{u_{k}} - p \frac{\partial \alpha_{k}}{\partial t} - p \nabla \cdot (\alpha_{k} \overset{\mathbf{r}}{u_{k}}) + I_{k} + \alpha_{k} \mathcal{Q}^{''}$$

where k = v, l, or d

The left hand sides of the equations are from timevariation, convection and diffusion of the dependent variables. The right hand sides are sources from phase change, phasic interaction and others.

3. Numerical Methods

3.1 General Transport equation

All the governing equations can be cast into the following integral form:

$$\frac{\partial}{\partial t}\int \rho\phi \,d\Omega + \frac{\partial}{\partial\tau}\int \rho\phi \,d\Omega + \int \rho\phi \overset{r}{u}\overset{r}{dA} - \int \Gamma \nabla\phi \,\overset{r}{dA} = \int S^{\phi} \,d\Omega \quad (2)$$

where ρ is a density of the fluid, ϕ is the dependent variable of the transport equation, $\frac{1}{u}$ is a velocity vector, Γ is a diffusion coefficient, for example, $\Gamma = \mu$ for the momentum equation. q_{ϕ} is a source term of the equation.

By the context of the dual-time delta formulation [3], the transport equation can be written as:

$$\begin{bmatrix} \frac{\rho\Omega}{\delta t} + \frac{\rho\Omega}{\delta \tau} + \sum_{f} \left(\frac{dC_{f}}{d\phi} - \frac{dD_{f}}{d\phi} \right) - \Omega \frac{dS^{\phi}}{d\phi} \end{bmatrix}_{c0}^{n+1,m} \delta\phi_{c0}^{n+1,m}$$

$$+ \sum_{f} \left(\frac{dC_{f}}{d\phi} - \frac{dD_{f}}{d\phi} \right)_{cj}^{n+1,m} \delta\phi_{cj}^{n+1,m}$$

$$= -\frac{\Omega_{c0}}{\delta t} \left[(\rho\phi)^{n+1,m} - (\rho\phi)^{n} \right]_{c0} - \sum_{f} (C_{f}^{n+1,m} - D_{f}^{n+1,m}) + \Omega_{c0} S_{c0}^{\phi,n+1,m}$$
(3)

3.2 Momentum Equation

The inter-phasic momentum transfers such as a drag between the phases are very strong in multi-phase flows. These terms are treated in a point-implicit manner. By doing this, the momentum equations are coupled among phases in each Cartesian coordinate direction.

$$\begin{bmatrix} A_{v_{v,c0}}^{u} & A_{v_{d,c0}}^{u} & A_{v_{d,c0}}^{u} \\ A_{iv,c0}^{u} & A_{il,c0}^{u} & A_{id,c0}^{u} \\ A_{dv,c0}^{u} & A_{dl,c0}^{u} & A_{dd,c0}^{u} \end{bmatrix} \begin{bmatrix} \delta u_{i,c1}^{n+l,*} \\ \delta u_{i,c0}^{n+l,*} \\ \delta u_{d,c0}^{n+l,*} \end{bmatrix} + \sum_{f(c)} \begin{bmatrix} A_{v,cj}^{u} & 0 & 0 \\ 0 & A_{l,cj}^{u} & 0 \\ 0 & 0 & A_{d,cj}^{u} \end{bmatrix} \begin{bmatrix} \delta u_{i,c1}^{n+l,*} \\ \delta u_{i,cj}^{n+l,*} \end{bmatrix} = \begin{bmatrix} B_{v,c0}^{v} \\ B_{l,c0}^{u} \end{bmatrix} - \begin{bmatrix} \alpha_{l}^{n+l,m} \\ \alpha_{l}^{n+l,m} \\ \alpha_{d}^{n+l,m} \end{bmatrix} \left(\Omega \frac{dp}{dx} \right)_{c0}^{n+l,m}$$
(4)

Eq. (4) is the discretized momentum equations of the three-phases in x-direction for a cell c0.

3.3 Pressure Correction Equation

The pressure correction equation for the three-field model can be obtained by summing the three mass conservation equations.

$$\sum_{k=v,l,d} 1/\rho_{k,ref} \left\{ \Omega \frac{\partial}{\partial t} (\alpha_k \rho_k) + \sum_f (\alpha_k \rho_k u_k A)_f - \Omega S_k^{\alpha} \right\} = 0 \quad (5)$$

To normalize the mass errors from each phase, the phasic mass equation is divided by its reference density before being summed to one. This normalizing scheme reduces the biased effect from the heavy phase. The velocity and density of each phase are split into expect and correction values as follows.

$$\rho_k^* = \rho_k^m + \rho_k' \qquad u_k^{m+1} = u_k^* + u_k' \tag{6}$$

The corrections of the density and velocity are related to the pressure correction based on the context of the SIMPLE algorithm.

$$\rho'_{k} = \frac{d\rho_{k}}{dp} p' = C_{p,k} p' \quad \tilde{u}'_{k,c0} = -A^{p}_{k,c0} \left(\nabla p'\right)_{c0}$$
(7)

By using the eq. (7), the summed mass equation is changed to the pressure correction.

$$\sum_{k=v,l,d} \frac{1}{\rho_{k,ref}} \left\{ \frac{\Omega}{\delta t} \alpha_{k}^{n+1,m} C_{p,k} p' + \sum_{f} (\alpha_{k}^{n+1,m} C_{p,k} p' U_{k}^{n+1,*})_{f} - \sum_{f} (\alpha_{k}^{n+1,m} \rho_{k}^{n+1,m} A_{k}^{p} \nabla p' A_{f})_{f} \right. \\ = -\sum_{k=v,l,d} \frac{1}{\rho_{k,ref}} \left\{ \frac{\Omega}{\delta t} (\alpha_{k}^{n+1,m} \rho_{k}^{n+1,m} - \alpha_{k}^{n} \rho_{k}^{n}) + \sum_{f} (\alpha_{k}^{n+1,m} \rho_{k}^{n+1,m} U_{k}^{n+1,*})_{f} - \Omega S_{k}^{\alpha} \right\}$$
(8)

4. Numerical Results

The numerical method proposed in this study was validated by solving a phasic separation in a square cavity. Initially, vapor and liquid are equally mixed and distributed in the cavity. When time goes by, the two phases are separated by the density difference under gravity. Fig. 1 shows the phasic volume fractions and the induced velocity fields by the phase separation at each time.



Fig. 1 Phasic distributions and velocity fields, left: liquid, right: vapor, top: t=2s, middle: t=4s, bottom: t=10s

5. Conclusion

A two-phase three-field model was implemented on an unstructured-mesh SIMPLE solver. In this study, it was found that the numerical method is promising for a two-phase flow analysis.

REFERENCES

- A. Kumbaro, V. Seignole, "Numerical Modeling of Two-Phase Flows Using Advanced Two Fluid Systems", ICONE-10, 2002
- [2] J. J. Jeong et. al, "Hydrodynamic Solver for a Transient, Two-Fluid, Three-Field Model on Unstructured Grids", KSCFE, vol. 12, No. 4, 2007
- [3] J. Kim et. al, "Delta-formulation of a Segregated Navier-Stokes Solver with dual-time Integration", KSCFE fall, 2006