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Simulation of industrial multiphase flows

공학적 관점에서의 다상유동 문제의 수치해석

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Abstract

In many industrial applications, multiphase flow analysis is the norm rather than an exception as compared to more-conventional single-phase investigation. This paper describes the implementation of the multiphase flow simulation capability in the general purpose CFD software AVL FIRE/SWIFT. The governing equations are discretized based on a finite volume method (FVM) suitable for very complex geometry. The pressure field is obtained using the SIMPLE algorithm. Depending on the characteristics of the multiphase flow to be examined, the user can choose either the two-fluid model or an explicit interface-tracking model based on the Volume-of-Fluid approach. For truly "multi"-phase flow problems, it is also possible to apply a hybrid model where certain phases are explicitly tracked while the other phases are handled by the two fluid model. In order to demonstrate the capability of the method, applications to the Taylor bubble flow simulations are presented.

1. INTRODUCTION

As industry constantly seeks for more efficient design and production methodology, numerical simulations play a crucial role to examine the multiphase flows involved in many engineering processes.

In general, numerical approaches for industrial multiphase flows are divided into two major categories: 1) Two-fluid (or multi-fluid) models based on averaging concepts that require additional modeling for the closure of the governing equations; 2) Interface tracking (or capturing) methods based on direct numerical simulation that require an accurate representation of the interface on the computational grid and, therefore, are more computationally intensive.

In practice, the choice between the two approaches is made not only by considering the overall flow characteristics, but also by comparing the required spatial and temporal resolutions of the solution to the available computing resources.

We aimed to develop a robust, efficient numerical technique that enables simulations of practical multiphase flow problems with complex geometry. Special attention was paid to ensure that a wide range of multiphase flows can be handled effectively. To this end, we provide the user with a capability to switch between the two-fluid model and the Volume-of-Fluid (VOF) interface tracking model as necessary. It is also possible to apply a hybrid method that combines the two-fluid and the Volume-of-Fluid (VOF) interface tracking approaches. This feature is particularly attractive when relatively large-scale interfaces between different phase/fluids co-exist with much smaller-scale multiphase structures. Examples of such flows can be found in fuel spray injection, boiling in a channel and tank filling, to name a few.

In the next sections, we describe the mathematical basis of the numerical method, followed by an application example—the Taylor bubble flows.

2. MATHEMATICAL MODEL

We consider a multiphase flow and assume that all fluids are incompressible and Newtonian. We first describe the multi-fluid model and later discuss the modifications due to the incorporation of the Volume-of-Fluid (VOF) interface tracking method.

2.1 Multi-fluid Model

The mathematical fundamentals of the multi-fluid model can be found in Drew & Passman [1] and a comprehensive review is provided by Lahey & Drew [2]. We describe briefly our multi-fluid model implementation below:

Mass conservation of a single component in the multi-phase flow is equal to:

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$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \mathbf{v}_k = \sum_{l=1, l \neq k}^{N} \Gamma_{kl} \quad (1)$$

where α_k is k-th phase volume fraction, Γ_{kl} is the mass exchange term between the phase's k and l, and N is the number of phases tracked by the multi-fluid model.

Momentum conservation equation for k-th phase equals:

$$\frac{\partial \alpha_k \rho_k \mathbf{v}_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k = -\alpha_k \nabla p + \nabla \cdot \alpha_k (\boldsymbol{\tau}_k + \boldsymbol{\tau}_k^t) + \alpha_k \rho_k \mathbf{g} + \sum_{l=1, l \neq k}^{N} \mathbf{M}_{kl} + \sum_{l=1, l \neq k}^{N} \mathbf{v}_k \Gamma_{kl} \quad (2)$$

where $\boldsymbol{\tau}_k$ is shear stress due to the viscosity, and $\boldsymbol{\tau}_k^t$ is Reynolds stress. $\mathbf{M}_{kl}$ represents the interfacial momentum transfer between phase's k and l. In our implementation, it includes drag and turbulent dispersion forces:

$$\mathbf{M}_{kl} = C_D \frac{1}{8} \rho_k A_i''' |\mathbf{v}_r| \mathbf{v}_r + C_{TD} \rho_k k_k \nabla \alpha_l = -\mathbf{M}_{lk} \quad (3)$$

where A_i''' is interfacial area density, $\mathbf{v}_r$ is relative velocity, C_D is drag coefficient, and C_{TD} is turbulent dispersion coefficient. Assumed is uniform pressure field for all phases:

$$p_k = p, \quad k = 1,.., N \quad (4)$$

When turbulence effects need to be considered, the standard k-ε model is employed. Turbulence conservation equation is solved for each phase:

$$\frac{\partial \alpha_k \rho_k k_k}{\partial t} + \frac{\partial \alpha_k \rho_k k_k v_{k,l}}{\partial x_l} = \alpha_k \rho_k P_k + \frac{\partial}{\partial x_l}\left(\alpha_k \rho_k \frac{C_\mu}{\sigma_k} \frac{k_k^2}{\varepsilon_k} \frac{\partial k_k}{\partial x_l} \right) - \alpha_k \rho_k \varepsilon_k + \sum_{l=1, l \neq k}^{N} k_k \Gamma_{kl} \quad (5)$$

where P_k is the production term.

Turbulence dissipation equation equals:

$$\frac{\partial \alpha_k \rho_k \varepsilon_k}{\partial t} + \frac{\partial \alpha_k \rho_k \varepsilon_k v_{k,j}}{\partial x_j} = - \rho_k \alpha_k C_{\varepsilon 1} \frac{\overline{v'_{k,i} v'_{k,j}}}{k_k} \frac{\partial v_{k,i}}{\partial x_j} \varepsilon_k - \rho_k \alpha_k C_{\varepsilon 2} \frac{\varepsilon_k^{\,2}}{k_k} + \frac{\partial}{\partial x_j}\left(\rho_k \alpha_k \frac{C_\varepsilon k_k}{\varepsilon_k} \overline{v'_{k,j} v'_{k,l}} \frac{\partial \varepsilon_k}{\partial x_l} \right) + \sum_{l=1, l \neq k}^{N} \varepsilon_k \Gamma_{kl} \quad (6)$$

The closure coefficients for turbulence kinetic energy and turbulence dissipation equations are given in Table 1.

σ_k	σ_ε	σ_T	C_1	C_2	C_3	C_4	C_μ
1.0	1.3	0.9	1.44	1.92	1.44	-0.33	0.09

Table 1. Closure coefficients in the *k*-ε model.

Depending on the nature of the problem, further simplification can be made to the multi-fluid model described above: Certain phases may be grouped together so that they are homogenous in momentum (same velocity). For example, in a 5-phase problem, 3 of the phases may have indistinguishable velocity fields and hence they may be specified as homogenous in the momentum exchange. Since only one set of the momentum equations needs to be solved for all phases in the same homogeneous group, computing effort can be reduced substantially and also the simulation becomes more robust.

2.2 VOF Interface Tracking Model

When well-defined sharp interfaces between different phases (spanning more than a few grid points) are present in the computational domain, a numerical model based on the Volume-of-Fluid (VOF) method (Hirt & Nichols [3]) is adopted for explicit interface tracking. In this approach, the motion of the interface is tracked by the solution of a scalar transport equation for a phase-indicator field that is discontinuous at the interface and uniform elsewhere. Although most common VOF applications are two-phase flows, it is also valid for flows with multiple sharp interfaces.

In our implementation, we choose the volume fraction for a particular phase (say, the j-th phase) on either side of the sharp interface as the phase-indicator function. Then each computational cell has a value:

$$\alpha_j = \begin{cases} 1 & \text{if fully occupied by } j\text{-th phase} \\ 0 & \text{if not occupied by } j\text{-th phase} \end{cases} \quad (7)$$

and the tracked interface exists in the partially-filled cells (with a volume fraction between 0 and 1).

The governing equation for the volume fraction of the tracked phase can be written in the conservative form as:

$$\frac{\partial \alpha_j}{\partial t} + \nabla \cdot \alpha_j \mathbf{v}_j = 0 \quad \text{for } j = 1, \ldots\ldots, M \quad (8)$$

where M is the number of phases tracked by the VOF model.

The unique feature of the VOF model is in the treatment of the convection term in Eq. (8). To limit numerical diffusion, a special discretization scheme must be applied. In our implementation, a scheme developed for unstructured meshes with arbitrary shape (Ubbink & Issa [4]) is employed. Once the volume fraction field at the next time step is obtained using Eq. (8), the local mixture fluid properties are calculated for the entire computational domain using the volume fraction-weighted averaging (so-called "one-field formulation"). With the mixture properties, the same sets of the governing equations defined for single-phase flows can be used to determine the velocity field. Surface tension effects are included using the Continuum Surface Force (CSF) model (Brackbill et. al [5]).

2.3 Hybrid Model

The construction of the hybrid model is based on the observation that, for incompressible fluids, both Eqns. (1)

and (8) are equivalent (neglecting the mass exchange term). Consequently, the multi-fluid and the VOF models can be coupled through the common expression for mass conservation, Eq. (1). The only difference is in the handling of the convection term: the volume fraction fields for the VOF-phases are updated by using a special VOF differencing scheme, while those for the multi-fluid phases are obtained by an ordinary scheme such as upwind or central discretization. The overall mass conversation is satisfied by enforcing the compatibility condition: $\sum_{i=1}^{N+M}\alpha_i = 1$.

(9)

2.4 Flow solver implementation

The model described above has been implemented into the commercial CFD code AVL SWIFT/FIRE. The solution method is based on a fully conservative finite volume approach. All dependent variables, such as momentum, pressure, density, turbulence kinetic energy, dissipation rate, and passive scalar are evaluated at the cell center. The cell-face based connectivity and interpolation practices for gradients and cell-face values are introduced to accommodate an arbitrary number of cell faces.

With the exception of the volume fractions for VOF phases, the discretization of the governing equations is done in a usual way: A second-order midpoint rule is used for integral approximation. The convection is solved by a variety of differencing schemes (upwind, central differencing, MINMOD, and SMART) and a second order linear approximation for any value at the cell-face. A diffusion term is incorporated into the surface integral source after employment of the special interpolation practice. The rate of change is discretized by using implicit schemes, namely Euler implicit scheme and three time level implicit scheme of second order accuracy.

The overall solution procedure is iterative and is based on the Semi-Implicit Method for Pressure-Linked Equations algorithm (SIMPLE). For the solution of a linear system of equations, either a conjugate gradient type of solver or an Algebraic Multi Grid (AMG) solver is used.

3. APPLICATION EXAMPLE

In order to demonstrate the capability, the hybrid method was applied to a well-established multiphase flow example—a Taylor bubble (For details, see [6], [7] and the references cited therein).

First we consider a single air bubble moving in a vertical pipe (diameter D=0.0151m, height $H=9D$) filled with water. The initial gas bubble shape is a cylinder with diameter of 0.8D with hemispheres attached at both ends. We assumed that the flow is axisymmetric and laminar and all phases share the same velocity field. Note that these assumptions were made only for simplicity and the hybrid model can easily accommodate more general cases.

The fluid properties and the relevant non-dimensional numbers are summarized in Table 2.

ρ_l	ρ_g	μ_l	μ_g	σ	Eo	Mo
1311	1.22	0.01725	1.8×10^{-5}	0.076	38.54	1.5×10^{-6}

Table 2. Physical properties (in SI units) and non-dimensional numbers.

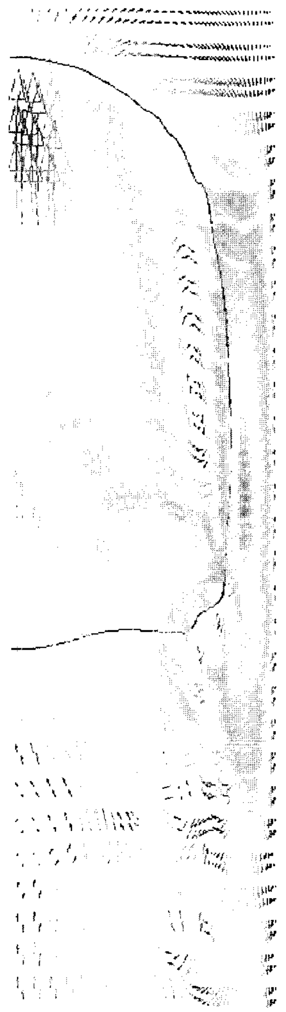

Figure 1. Velocity vector plot at t*=15.31. Black solid line is the bubble interface.

Figure 1 shows a typical flow pattern around the Taylor bubble obtained by applying a conventional pure VOF approach with 2 phases; no multi-fluid model was used in the simulation. The velocity plot clearly shows that gas-entrainment takes place due to the large velocity difference between the liquid slug front and the liquid film surrounding the Taylor bubble. Consequently, the accuracy of the VOF model prediction is compromised in the wake region due to the lack of sufficient grid resolution.

Figure 2 shows the result obtained using the hybrid approach. Here, the simulation starts in a similar way with two phases (phase 1: water, phase 2: air) tracked by the VOF model. The only change from the previous case is the addition of the third phase, whose initial volume fraction value is set to zero everywhere.

During the course of the simulation, interface diffusion is monitored and detected: When the air volume fractions both inside a particular cell and its closest neighboring cells are below a predefined value, the corresponding volume for phase-2 is transferred into phase-3 and handled with the multi-fluid model as a dispersed phase thereafter. The re-coalescence of the dispersed phase into the Taylor bubble was not considered, which is a reasonable assumption for the parameters considered. This simple technique is admittedly a heuristic approach to model the real entrainment process and will be replaced in the future by more sophisticated models based on first-order physical principles. However, the overall flow characteristics are simulated well.

Figure 2. Taylor bubble evolution using the hybrid model. Volume fraction field tracked by the multifluid model (phase 3) is plotted at four non-dimensional times (denoted by the numbers inside the frames). A white solid-line in each frame is an iso-contour of the air volume fraction (phase 2), tracked by the VOF model. The background fluid (phase 1) is water.

Figure 3. Taylor bubble in a small diameter pipe. The volume fraction field is plotted to show the bubble evolution.

In Figure 3, the evolution of Taylor bubble in a small diameter pipe (D=1.95mm) is presented. In this case, the bubble moves due to the inflow with a parabolic velocity profile entering the bottom boundary and the gravity is neglected. The Reynolds and the Weber numbers are 8.93 and 0.22, respectively. Since the entrainment is not significant, the bubble interface is tracked solely by the VOF model. After initial deformation, the bubble maintains a steady-state shape with a thin layer of liquid film between the wall and the bubble.

4. CONCLUSION

Presented was a numerical method for multiphase flows including a hybrid model which is suitable when interfaces with a range of spatial scales exist simultaneously in the computational domain. The method was applied to simulate the evolution of a Taylor bubble, which showed a promising result. More simulations of the Taylor bubble case with three-dimensional effects and advanced entrainment and re-coalescence models are in progress.

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