NASA CR-201983



# ATOMIZATION SIMULATIONS USING AN EULERIAN-VOF-LAGRANGIAN METHOD

Yen-Sen Chen, Huan-Min Shang and Paul Liaw
Engineering Sciences, Inc.
Huntsville, AL 35802

C. P. Chen
University of Alabama in Huntsville
Huntsville, AL 35899

## ABSTRACT

This paper summarizes the technical development and validation of a multiphase computational fluid dynamics (CFD) numerical method using the volume-of-fluid (VOF) model and a Lagrangian tracking model which can be employed to analyze general multiphase flow problems with free surface mechanism. The gas-liquid interface mass, momentum and energy conservations are modeled by continuum surface mechanisms. A new solution method is developed such that the present VOF model can be applied for all-speed flow regimes. The objectives of the present study are to develop and verify the fractional volume-of-fluid cell partitioning approach into a predictor-corrector algorithm and to demonstrate the effectiveness of the present innovative approach by simulating benchmark problems including the coaxial jet atomization.

## INTRODUCTION

The atomization and breakup processes of liquid fuel in many space transportation and propulsion systems are of vital importance to combustion performance and stability. Numerical modeling of these flows poses a significant challenge because it requires simultaneous resolutions of transient liquid-gas-droplets dynamics, and the flow regimes considered can range from incompressible to high-speed compressible flows. The flow-process modeling is further complicated by surface tension, interfacial heat and mass transfer, material property variation, spray formation and turbulence, and their interactions. It is the aim of this study that a general and robust design analysis tool will be available as a result of the incorporation of advanced numerical and physical models in a computational fluid dynamics flow solver.

Historically, developments of numerical methods for multiphase free surface flows were primarily aimed at incompressible flows utilizing the Volume of Fluid (VOF) method. [1,2]. These methods are often ineffective for high-speed, high-Reynolds-number flows. So far, multiphase free surface flows have not been considered in more general all-speed flow algorithms, with only a few recent exceptions [3,4,5]. In the ARICC-3D Code [3], the VOF method was implemented in the ALE-ICE (Arbitrary Lagrangian Eulerian-Implicit Continuous-fluid Eulerian method) algorithm for injector flow simulation with atomization. Due to the inefficiency of the ALE-ICE method, the ARICC-3D was found very time-consuming for multi-

* This work was sponsored by NASA-MSFC with Dr. T.S. Wang as technical monitor under contract NAS8-40148. Approval for public release; distribution is unlimited.

element computations. Recently, the ALE-ICE method was abandoned by the code developer in favor of the pressure-based SIMPLE algorithm [4]. In the RIPPLE computer program [5], only finite difference solutions to the incompressible Navier-Stokes equation are obtained on an Eulerian, rectangular mesh using a time-split two-step projection algorithm. Compressible fluids were not solved, while the surface tension is treated using a novel continuum surface force (CSF) model.

Based on a preliminary study presented last year [16], a unified multi-phase numerical method is developed. The gas-liquid interface mass, momentum and energy conservation properties are modeled by continuum surface mechanisms. A new solution method is developed such that the present VOF model can be applied for all-speed range flows. The objectives of the present study are: (a) to develop and verify the fractional volume-of-fluid (VOF) cell partitioning approach into a predictor-corrector algorithm to deal with multiphase (gas-liquid) free surface flow problems; (b) to implement the developed unified algorithm in a general purpose computational fluid dynamics (CFD) code, Finite Difference Navier-Stokes (FDNS), with numerical treatment of droplet dynamics models described in [6].

The main feature of the present method is to combine the novel feature of the Volume of Fluid (VOF) method and the Eulerian/Lagrangian method used in a pressure-based particulate two-phase flow solver [6, 9, 10] into a unified algorithm for efficient non-iterative, time-accurate calculations of multiphase free surface flows valid at all speeds. The proposed method reformulated the VOF equation to strongly couple two distinct phases (liquid and gas), and tracks droplets on a Lagrangian frame when spray model is required, using a unified predictor-corrector technique to account for the non-linear linkages through the convective contributions of VOF. The discontinuities within the sharp interface will be modeled as a volume force to avoid stiffness. Formations of droplets and tracking of droplet dynamics are handled through the same unified predictor-corrector procedure. Thus the new algorithm is non-iterative and is flexible in the handling of any general geometries with arbitrarily complex topology in free surfaces. The present method can also be applied for efficient steady state situations and can be implemented into any pressure-based methodology. For the purpose of algorithm development and validation, the proposed method will be implemented into a general purpose CFD code, Finite Difference Navier-Stokes FDNS [9,10], which has three dimensional and multi-zone capabilities.

## METHODOLOGY

### Governing Equation

Conventionally, there have been some successful numerical algorithms for performing multiphase flow calculations involving free interfaces. In general, two basic approaches can be identified. One is based on the Lagrangian method and the other on the Eulerian frame work. The Lagrangian approach is to conform a mesh system with the sharp interface between gas and liquid and to track the movement of the interface according to sets of simplified equations governing the liquid and gas motions separately [8]. The entire Lagrangian grid network moves with the free surface which makes the grid generation or remeshing procedure very complex and CPU intensive. In the Eulerian approach, a fixed mesh system is used to resolve the sharp interface by the concept of a fractional volume of fluid (VOF) [11]. The second approach is more flexible and efficient in that it allows the resolution of the free surface to become part of the solution. The physical processes across the sharp interface such as surface tension forces, droplet or wave breakup, interphase mass transfer and condensation/vaporization, etc. can be modeled through the concept of continuum surface force (CSF) method [7] or by the method of

surface reconstruction as used in the ARICC3D code [4], SOLA-VOF code [1]. The CSF method is adopted in the present model for its generality and computational efficiency, especially for 3-dimensional computations.

Traditionally, VOF methods are mainly developed and used for low-speed flows such that incompressibility can be assumed. The incompressible flow assumption has limited their capability. To generalize, the present formulation is based on compressible flow governing equations. The forms of the equations are then continuously reduced to their incompressible forms according to the local flow conditions and the VOF solutions. This is the uniqueness of the present method. To illustrate this, the density-weighted averaged conservation equation of mass, Navier-Stokes, and scalar variables in an Eulerian frame work can be written as:

$$\frac{\partial \rho_m}{\partial t}+\frac{\partial \rho_m\left(u-u_g\right)_j}{\partial x_j}=S_{mp}$$

$$\frac{\partial \rho_m u_i}{\partial t}+\frac{\partial \rho_m\left(u-u_g\right)_j u_i}{\partial x_j}=-\frac{\partial p}{\partial x_i}-\frac{\partial}{\partial x_j}\left(\rho\overline{u'_i u'_j}\right)+S_{up} \qquad (1)$$

$$\frac{\partial \rho_m \phi}{\partial t}+\frac{\partial \rho_m\left(u-u_g\right)_j \phi}{\partial x_j}=-\frac{\partial}{\partial x_j}\left(\rho\overline{u'_j \phi'}\right)+S_\phi+S_{\phi p}$$

The VOF transport equation is given below.

$$\frac{\partial \alpha}{\partial t}+\left(u-u_g\right)_i\frac{\partial \alpha}{\partial x_i}=S_\alpha \qquad (2)$$

where $\alpha = 1$ stands for liquid and $\alpha = 0$ is for gas. The interface is located at $1 > \alpha > 0$. $S_\alpha$ represents the volume transfer rate across the two-phase boundaries. And,

$$\rho_m=(1-\alpha)\rho_g+\alpha\rho_l$$

where $\rho_m$ denotes the time-mean density of the mixture, $\rho_g$ and $\rho_l$ denote gas and liquid density respectively, $u_i$ and $u'_i$ are the i-component of the density-weighted mean and fluctuating part of the instantaneous velocity, $\phi$ and $\phi'$ are the density-weighted mean and fluctuating part of the instantaneous scalar quantities including the species concentrations, turbulence quantities and the gas mixture enthalpy, p is the mean pressure, S represents sources terms due to mass transfer, momentum transfer, species production, etc. $u_g$ represents the grid speed components used to simulate moving domain effects. Detailed expressions of these source terms can be found in Refs. 9 and 10. In the present study, the turbulent correlation terms, $\overline{u'_i u'_j}$ and $\overline{u'_i \phi'}$, are modeled by the two-equation turbulence closure models [12]. For a given solution of $\alpha$ field, equation (1) can be rewritten as the following form to maintain accurate transient from the gas phase flowfield to the liquid phase flow solution through the interface.

$$\frac{\partial \rho_m \phi}{\partial t}+\frac{\partial \rho_m\left(u-u_g\right)_i \phi}{\partial x_i}=S_\phi, \quad \alpha<0.01 \quad \text{--------} \quad \text{for compressible gas}$$

$$\rho_m\frac{\partial \phi}{\partial t}+\rho_m\left(u-u_g\right)_i\frac{\partial \phi}{\partial x_i}=S_\phi, \quad \alpha\geq 0.01 \quad \text{--------} \quad \text{for interface and liquid}$$

### Interface Resolution Model

The numerical accuracy of the VOF method depends highly on the interface resolution. To prevent the solution from becoming too smearing due to numerical diffusion, a compression procedure is developed to perform VOF interface rescaling such that the average thickness within the interface ($0.1 < \alpha < 0.9$) is kept constant through out the computation. The interface $\alpha$ solution compression procedure is expressed as:

$$\alpha_{new} = Max\left\{0, Min\left[1, 0.5 + f\left(\alpha_{old} - 0.5\right)\right]\right\}$$

and

$$f = \frac{(Interface\ \ Thickness)_{new}}{(Interface\ \ Thickness)_{initial}}$$

### General Continuum Surface Tension Force Model

The surface tension forces in the continuum surface force model are formulated as continuous body forces across the interface. These forces can be written as,

$$F_x = -\sigma\left(\nabla \hat{n}\right)\alpha_x$$

$$F_y = -\sigma\left(\nabla \hat{n}\right)\alpha_y + \left(\frac{|\alpha_y|}{y}\right)_{for\ 2D\ axisymetric\ only}$$

$$F_z = -\sigma\left(\nabla \hat{n}\right)\alpha_z\ ,\quad ---\ for\ 3D\ case\ only$$

where $\sigma$ = surface tension coefficient and $\nabla \hat{n} = \hat{\alpha}_{xx} + \hat{\alpha}_{yy} + \hat{\alpha}_{zz}$

### Interface Mass Transfer Model

To simulate the mass transfer effects along the interface of the gas and liquid phases, the source term of Eq. (2) is modeled. The sign and magnitude of the VOF source term, $S_\alpha$ in Eq. (2), depend on the physical processes involved. For spray atomization applications, for instance, it would represent the volume stripping rate which can be modeled by atomization correlations. For spray coating, condensation and chemical vapor deposition processes, on the other hand, positive volume flow rates would result.

There are basically two ways of modeling the VOF source term. One method is to treat the inter-phase volume flow rate as convection process along the interface. That is,

$$S_\alpha = V_s \cdot \nabla\alpha$$

where $V_s$ denotes the volume exchange velocity. This method allows the source term and the convection terms be combined so that the source effects are handled implicitly. However, the accuracy of this approach depends entirely on the assignment of the volume exchange velocity. Vectors directly normal to the interface do not always guarantee good solution.

The second approach, which is the most straight forward treatment, solve the VOF equation with the source term specified explicitly. This approach is general and provides good numerical accuracy. The only drawback of this method is the possible numerical instability related to high volume flow rates. Time step size must be small enough in order to solve the VOF equation with large source term.

**Numerical Algorithm**

Time-Marching Scheme

For simplicity, the density-weighted conservation equation of mass, momentum, enthalpy, and scalar variables in an Eulerian coordinate can be written as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i) = S_m$$

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i \phi) = S_\phi$$

where $S_\phi$ consists of the diffusion fluxes and the source terms. Using general $\theta$ method for temporal discretization, the above transport equations are discretized as:

$$(\rho^{n+1} - \rho^n)/\Delta t + \theta\,(\rho U)_x^{n+1} + (1-\theta)(\rho U)_x^n = \theta\, S_m^{n+1} + (1-\theta) S_m^n$$

$$\left[(\rho\phi)^{n+1} - (\rho\phi)^n\right]/\Delta t + \theta\,(\rho U\phi)_x^{n+1} + (1-\theta)(\rho U\phi)_x^n = \theta\, S_\phi^{n+1} + (1-\theta) S_\phi^n$$

where $\theta$ = 1/2 represent the time-centered Crank-Nicholson scheme which is second-order accurate in time. This scheme is used in the present study. By substituting the continuity equation into the scalar transport equation, the delta form of the advection equation of the scalar transport equation is obtained:

$$\left[\frac{\rho^n}{\Delta t} - (1-\theta)(\rho U)_x^n\right]\Delta\phi + \theta\left[(\rho U)^n + \Delta(\rho U)\right]\Delta\phi_x$$

$$= -\left[(\rho U)^n + \Delta(\rho U)\right]\phi_x + (1-\theta)\Delta(\rho U)\phi_x + \theta\, S_\phi^{n+1} + (1-\theta) S_\phi^n$$

The predictor and corrector of the above equation are then written as:

$$\left[\frac{\rho^n}{\Delta t} - (1-\theta)(\rho U)_x^n\right]\Delta\phi + \theta\left[(\rho U)^n + \Delta(\rho U)\right]\Delta\phi_x$$

$$= -\left[(\rho U)^n + \Delta(\rho U)\right]\phi_x + (1-\theta)\Delta(\rho U)\phi_x + S_\phi^n$$

and

$$\left[\frac{\rho^n}{\Delta t} - (1-\theta)(\rho U)_x^n\right]\phi' + \theta\left[(\rho U)^n + \Delta(\rho U)\right]\phi'_x = \theta\, S'_\phi$$

In the corrector stage, pressure field, velocity vectors, density field and enthalpy are updated by solving the pressure correction equation and the scalar correction equations. For wave propagation problems, 3 to 4 correctors are sufficient for convergence.

High-Order TVD Scheme

In the present study all test cases were analyze with a high-order upwind TVD Scheme. Only the convection terms are modeled using the TVD flux limiters. The convection terms of the governing equations can be expressed by finite difference approximation as:

$$\frac{\partial F}{\partial \xi} = f_{i+1/2} - f_{i-1/2} + h_{i+1/2} - h_{i-1/2}$$

where f and h represent first-order fluxes and TVD flux limiters respectively. The TVD flux limiters are functioned as anti-diffusion terms to recover the scheme to high-order accuracy. The first-order fluxes and the TVD flux limiters are given below.

$$f_{i+1/2} = \max\left\{0,(\rho U)_{i+1/2}\right\}\phi_i + \max\left\{0,-(\rho U)_{i+1/2}\right\}\phi_{i+1}$$

$$h_{i+1/2} = \begin{cases} \frac{1}{4}|\rho U|_{i+1/2}\left\{d\phi^{+}_{i+1/2} + d\phi^{-}_{i-1/2} + \alpha\left(d\phi^{+}_{i+1/2} - d\phi^{-}_{i-1/2}\right)\right\}, U \geq 0 \\ \frac{1}{4}|\rho U|_{i+1/2}\left\{d\phi^{-}_{i+1/2} + d\phi^{+}_{i+3/2} + \alpha\left(d\phi^{-}_{i+1/2} - d\phi^{+}_{i+3/2}\right)\right\}, U < 0 \end{cases}$$

where the minmod functions in the TVD flux limiters are written as:

$$d\phi^{\pm}_{i+1/2} = sign\left(\Delta\phi_{i+1/2}\right)\max\left\{0,\min\left[\left|\Delta\phi_{i+1/2}\right|,\beta\ sign\left(\Delta\phi_{i+1/2}\right)\Delta\phi_{i+1/2\mp1}\right]\right\}$$

The order of accuracy of this scheme is determined by the parameters $\alpha$ and $\beta$. Only the second-order and third-order upwind schemes were used in this study. That is,

$$\alpha = \begin{cases} -1, & 2nd-order\ upwind \\ +\frac{1}{3}, & 3rd-order\ upwind \end{cases}$$

$$\beta = Compression-Factor = \frac{3-\alpha}{1-\alpha}$$

The compression factor, $\beta$, is used to sharpen the contact discontinuities and slip streams for better wave tracking.

## VALIDATIONS

### Microgravity Fluid Tank Test Cases

To validate the present VOF method within the compressible and incompressible flow solver, some fluid tank benchmark test cases were investigated and compared with close form solutions. The key mechanisms involved here are the surface tension forces and the effects of wall contact angle. The liquid surface tension forces are modeled using the proposed continuum surface force (CSF) model and the wall contact angles are provided by the material properties and through the use of Young's equation.

Rotating Ethanol Tank:

In this test case, a rotating cylindrical ethanol tank (46.95% full) with radius of 3 cm and height of 2 cm was simulated. The rotational speed of the tank is 10 rpm. The surface tension coefficient of ethanol and the level of gravity force ($g/g_0$) are $2.28\times10^{-2}$ and $10^{-3}$ N/m respectively. A grid size of 31×31 with near wall grid clustering was employed for the computation. 2,000 time steps with a time step size of 2.0 were required for the surface waves to subside and reach a steady state solution. Figure 1 shows the predicted flow field and liquid surface shape and comparison with close form solution. Good agreement is reveal in the data comparison.

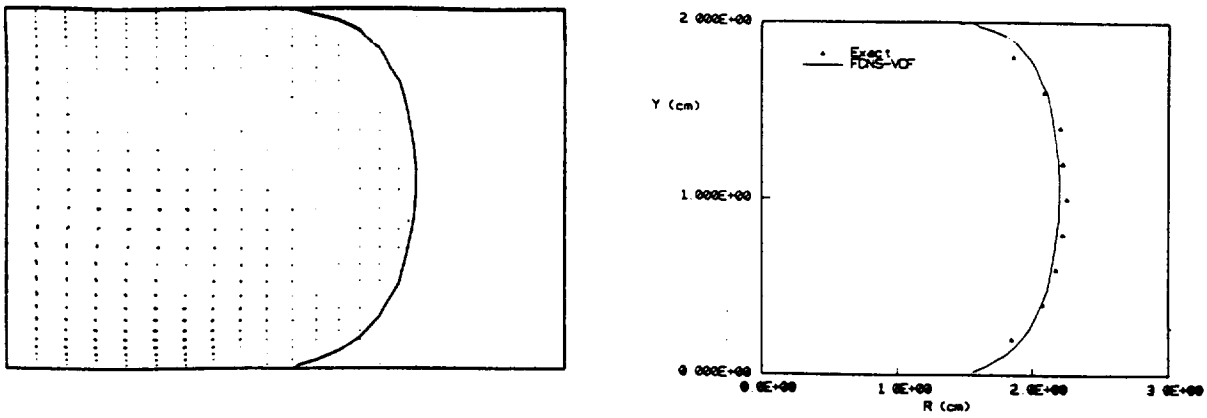


Figure 1. Rotating ethanol tank: $10^{-3}$ $g_0$ and 10 rpm.

Rotating Liquid Helium Tank:

In this test case, a rotating cylindrical helium tank (50% full) with inner and outer radii of 18.48 cm and 77.48 cm respectively, and height of 136 cm was investigated. The rotational speed of the tank is 1 rpm. The surface tension coefficient of helium (normal fluid) at 1.5 degree K and the level of gravity force ($g/g_0$) are $3.319\times10^{-4}$ N/m and $10^{-6}$ respectively. A grid size of 31×31 with near wall grid clustering was employed for the computation. 3,000 time steps with a time step size of 5.0 were required for the surface waves to subside and reach a steady state solution. Figure 2 shows the predicted flow field and liquid surface shape and comparison with close form solution. Good agreement is reveal in the data comparison.

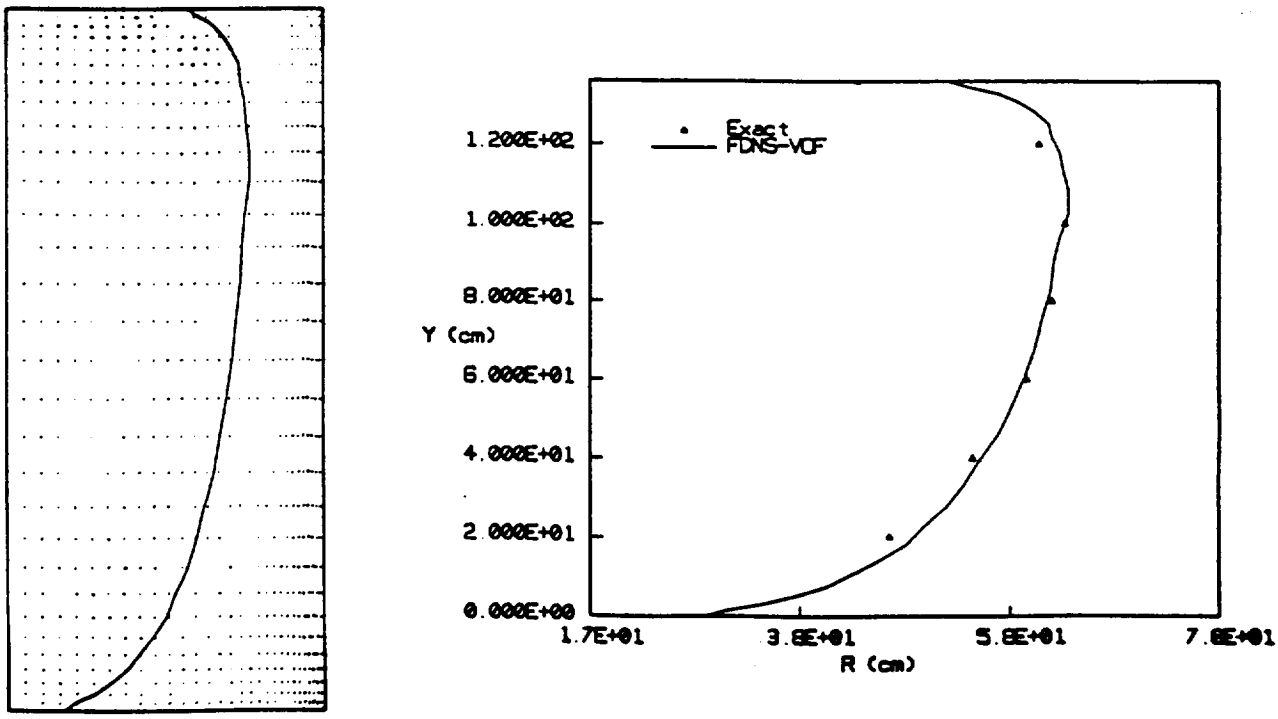


Figure 2. Rotating L-He tank: $10^{-6}$ $g_0$ and 1 rpm.

Cryogenic Liquid Helium Fluid Tank:

The working fluid and fluid properties of this test case is identical to that of the case 2 above. A dewar helium tank (with inner and outer radii of 12 cm and 70 cm respectively and height of 150 cm) under $10^{-7}$ $g_0$ and 0.1 rpm operating condition was tested. This case also provides a validation test of the surface tension force model for non-orthogonal grid systems. A steady state solution was obtained in 3,000 time steps with a time step size of 5.0. Figure 3 shows the predicted liquid surface shape and flow field. This solution is in good agreement with the numerical solution presented in Ref. 14.

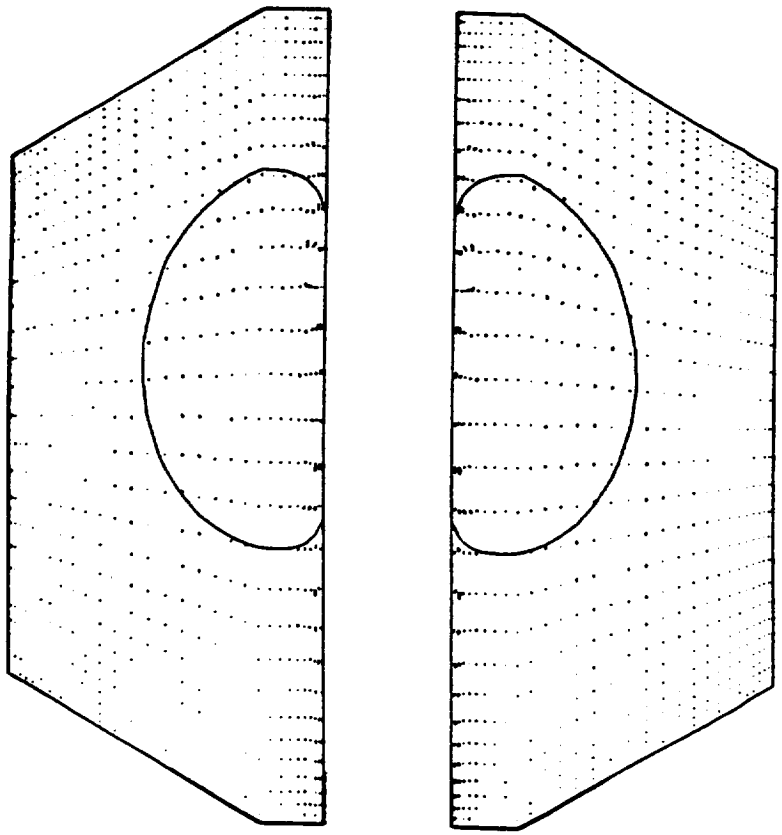

Figure 3. Rotating dewar solution: $10^{-7}$ $g_0$ and 0.1 rpm.

Rising Air Bubble in a Tank:

In this simulation, a spherical air bubble with radius of 20 cm was released at the center of a tank under $1g_0$ room temperature conditions. A 31×31 grid with time step size of 0.1 was used in the computation. This case is used to check the correctness of the pressure solutions across the interface and inside the bubble. Results of the predicted liquid interface, flowfield and pressure field for time level of 0.5 sec and 0.7 sec are given in Figure 4. It is clear that the predicted pressure inside the bubble stay almost constant and the shape of the pressure contour follows that of the bubble boundary. This simulation is considered to be physically correct.

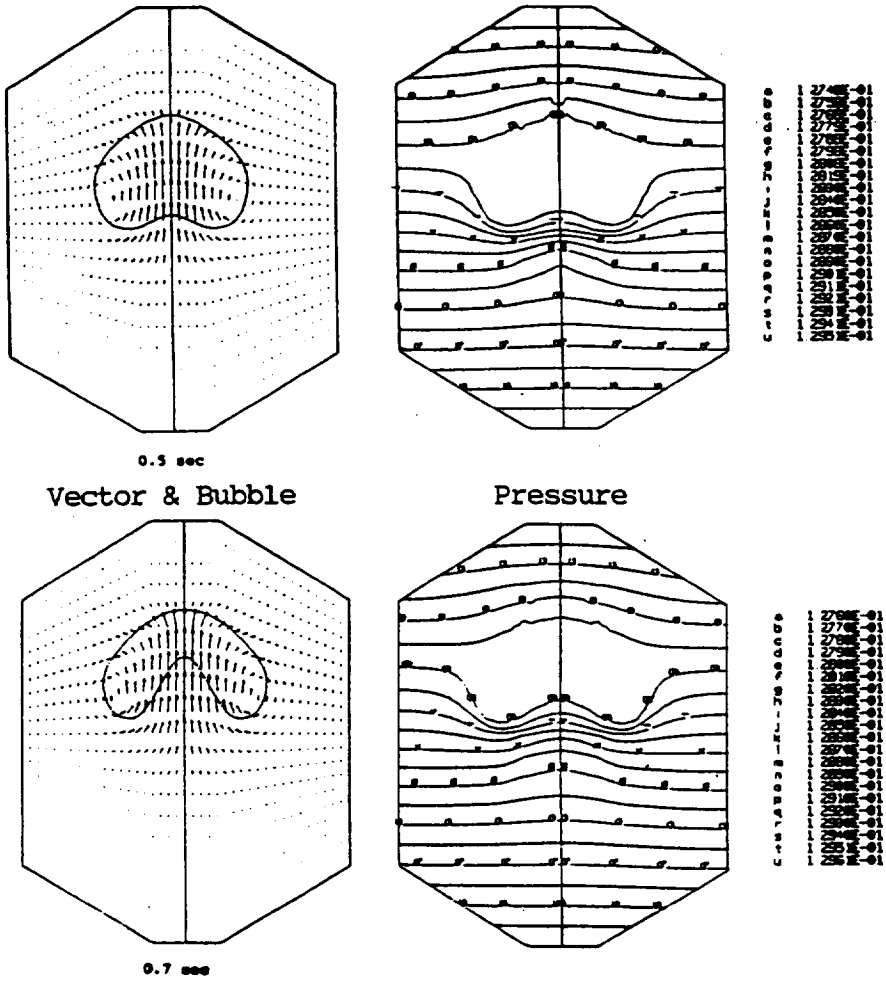


Figure 4. Rising air bubble simulation: $1g_0$ conditions.

**Coaxial Liquid Jet Atomization**

A cold flow case of coaxial liquid jet atomization reported by Liang and Schuman [15] is employed to test the current numerical methodology. Figure 5 shows the injector configuration. We use our unstructured grid code to simulate this multi-flow passage problem and expect to simulate multi-injector combustion applications by taking its advantage of grids flexibility for complex combustor geometry. In the current stage, the breakup rate is fixed as 10% of the liquid jet velocity and the droplet Sauter mean diameter is 100μm with Rosin-Rammler distribution. This restriction can be removed by using the wave instability model of Reitz et al. [17].

$H_2O$ and $CO_2$ are used as the liquid and gas in this study with injection velocity 12.14 m/s and 166.4 m/s respectively. 100 time steps are executed without injecting of particle but with liquid jet breakup. After that we ran another 50 time steps with particle injection from the surface and smaller time-step size (20μs). Figure 6 shows the velocity vectors and liquid core. Liquid jet velocity decreases due to the nozzle expansion and then is accelerated by the large slip velocity of gas phase. The numerical model is stable even for large time-step size and incompressible (liquid) /compressible (gas) flow situation. Figure 7 presents the particle trajectories at time = 1 ms. Particle turbulent dispersion effect has been included and large particle dispersion is shown due to high turbulent intensity of gas phase. The numerical prediction looks reasonable for the main flow feature. Further comparisons with benchmark data from Penn. State University are currently underway.

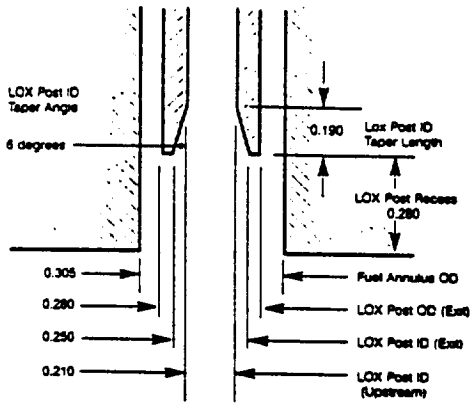


Figure 5. Schematic of coaxial injector configuration.

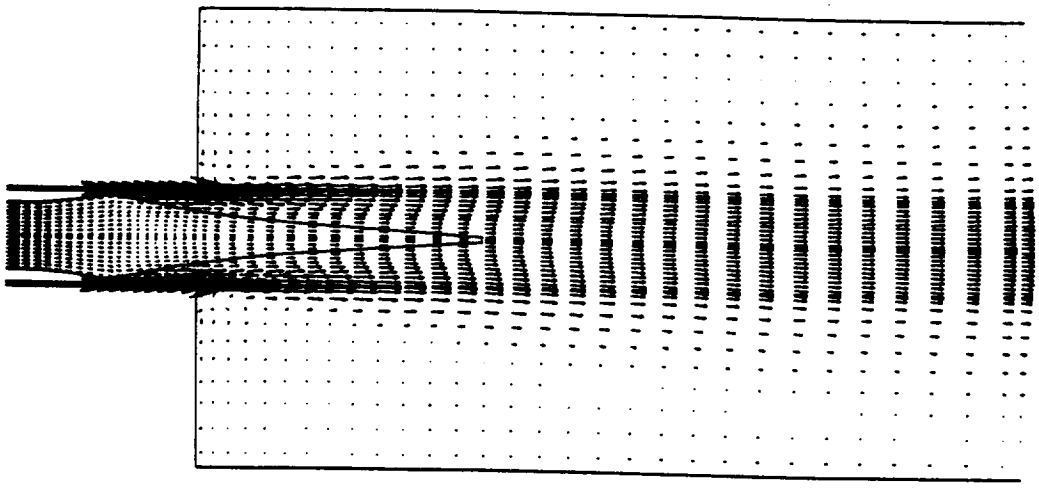

Figure 6. Velocity vector and liquid core.

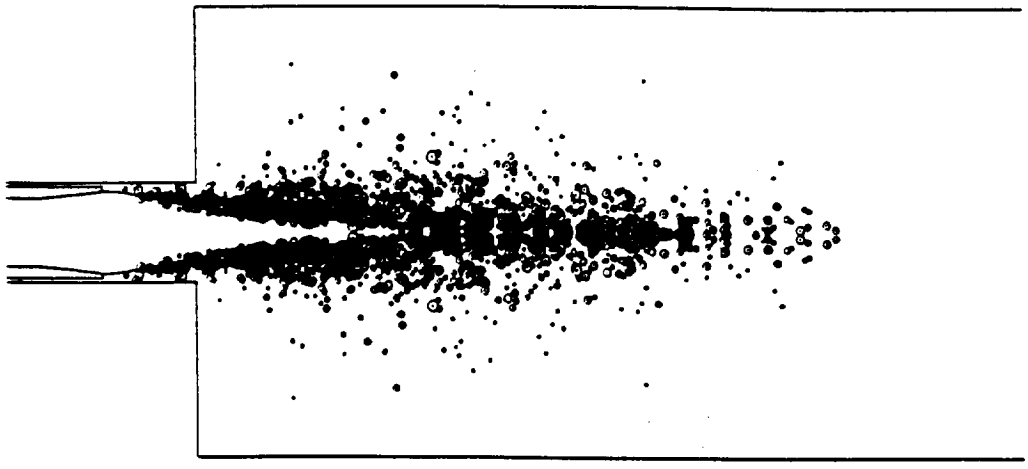

Figure 7. Particle trajectories at t = 1 ms.

## CONCLUSIONS

This paper summarizes the technical development and validation of a unified multiphase computational fluid dynamics (CFD) numerical method using volume-of-fluid (VOF) model which can be employed to analyze general multiphase flow problems with free surface mechanism. A time-accurate multiphase viscous flow solution method has been developed and validated with a wide range of benchmark test cases including the coaxial jet atomization. The gas-liquid interface mass, momentum and energy conservation properties are modeled by continuum surface mechanisms. A new solution method is developed such that the present VOF model can be applied for all-speed flow regimes. The objectives of the present study are to develop and verify the fractional volume-of-fluid cell partitioning approach into a predictor-corrector algorithm to deal with multiphase (gas-liquid) free surface flow problems; and to couple this unified algorithm with a non-iterative Lagrangian model. The successful implementation of this study will provide a reliable numerical model for the multiphase flow analysis as well as the fundamental building block for a analytical tool which may lead us toward the understanding of complex multiphase flow physics that is sometimes hard to visualize experimentally.

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