Application of Level Set Method to Analysis 2-D Two Phase Flow

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Abstract

Multi-phase fluid flows can be observed almost everywhere in nature and have a wide of range applications in engineering and natural processes such as atomization of jets and sprays, breaking waves, emulsions, boiling phenomenon, ship hydrodynamics, waterfalls and bubbly motion in cooling towers of nuclear power plants etc. In this paper, a physically possible mass conservative level set method of COMSOL multi-physics software has been illustrated to numerically investigate multi-phase fluid flow problem with and without considering surface tension concentrated on the interface. Here, the interface is represented by 0.5 iso- contour of the level set function ϕ where the value of ϕ is zero for the fluid inside the interface and 1 for the fluid outside the interface. In order to preserve the mass of the individual fluid phase present in actual physical problem, re- initialization procedure is made integral to the level set advection equation which is also known as governing equation of the dynamically evolving moving interface to keep the thickness (i.e. ϵ) of the interface constant across which the level set function ϕ varies smoothly from 0 to 1.The re-initialization process which is also called intermediate step consists of an artificial compressive flux try to compress the interface when its width is enhanced by the diffusion term, thus they are acting in opposite sense. When these two terms are in equilibrium then only finite thickness of the moving interface (i.e. ϵ) will be obtained. "P1+P1" discretization scheme is employed to discretize the incompressible Navier stokes equation whereas "linear" discretization technique is implemented to discretize the governing equation for the dynamically evolving interface. Single bubble rising problem in a matrix involving large density ratio (i.e. 1000) with and without considering surface tension have been numerically investigated using the proposed physically possible mass conservative level set method. However, transient evolution of a single bubble in a horizontal developing flow field without considering surface tension has also been numerically simulated to illustrate the robustness of this proposed numerical method. In all these case studies excellent mass conservation of the secondary fluid i.e. the bubble has been reported by using the proposed mass conservative level set method. Few benchmark incompressible two-phase flow problems in a rectangular geometry which includes merging of two-bubble having same density in a matrix with and without considering surface tension and rising of a single bubble involving different density ratios, viscosity ratios and also different magnitude of surface tension have been numerically computed for the purpose of proposed model validation.

Keywords: insert keyword

Introduction

Multi-phase fluid flows can be observed almost everywhere in nature and have a wide of range applications in engineering and natural processes such as atomization of jets and sprays, breaking waves, emulsions, boiling phenomenon, ship hydrodynamics, waterfalls and bubbly motion in cooling towers of nuclear power plants etc. These flows not only involve fluids with distinct physical properties but also complex interfacial motion between them with sharp changes in properties across the interface. Experimental investigation of this type of problems is difficult as well as expensive and that's why numerical methods are open used by researcher to analyze aforementioned problems. Discontinuities at the interface and the inherent multi scale nature of two-phase fluid flow problems throw numerous challenges to computational scientists and researchers across the globe. Recently, effect of large density ratio and high Reynolds number on multi- phase flow problem [37] has been

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numerically computed. In literature, two types of approaches have been found to handle the two-phase flow problems, namely the Front capturing method (Eulerian framework) [1] and the Front tracking method (Lagrangian framework) [2]. The front-tracking Method works well for multi-phase flow problems without any complex topological changes. In contrast, the front-capturing Method works well for multi-phase flow with complex topological changes. Front capturing methods are broadly classified into different categories such as a Volume of fluid (VOF) method, a Level Set Method (LS), a Phase Field Method (FP), and Hybrid Methods Such as a Coupled Level Set and Volume of Fluid method (CLSVOF) and a Coupled Volume of Fluid and Level Set Method (VOFSET), where the two methods are combined to have the advantages of both methods. Level Set method (LS) and Volume of Fluid (VOF)method are the two most widely used methods to handle interfacial flow problems among all front capturing methods.

In the Volume of Fluid Method, the complex interfacial motion of multi-phase flow problems is addressed by using the volume fraction function of one fluid in each computational cell which is later defined as the colour function. This method was first introduced by Hirt and Nichols [3] and they emphasized the need for numerical stability for accurate calculations and accordingly the choice of mesh increment, time increment, and upstream differencing parameters to prevent numerical instabilities were also included there. Although the VOF method is globally mass conserving and preserving the volume fraction of each phase near the interface, however, it suffers a lot when it comes to estimating surface tension and curvature/ normal to the interface. The interface reconstruction problem of the Volume of fluid method is overcome by introducing different variants of the VOF method [18], where the comparison of all variants is done in the CLSVOF (coupled level set and Volume of Fluid) Framework. Deviating from the above, Xiaosong et.al [21] introduced a new numerical method based on VOF and immersed boundary method to solve the two-phase flow problems involving complex geometries. Recently Faroog et.al [29] has introduced an improved version of the Volume of Fluid method for numerical modelling of multi-phase flows and transport problems where the pressure-velocity coupling is handled using a new algorithm called PISOR (Revised version of the PISO algorithm).

The Level Set Method was first introduced in 1987 by Osher and Sethian [2] for numerical modelling of dynamically evolving interfaces, which is based on the Eulerian framework of fluid dynamics, where the interface is defined as the zero- contour of the level set function. Level Set function is nothing but a scalar function and it is defined as the signed normal distance function from the pertinent location of the interface. One of the major reasons for using the Level Set method is that it can accurately calculate interface curvature and automatically deal with problems involving topology changes such as merging or breaking of bubbles. Despite this great advantage, the main problem of the level Set method is that it is not conservative. In the case of incompressible immiscible two-phase flow, the volume of the individual phase is constant but there is loss or gain of mass of the individual phase during numerical simulation using the level set method, which is physically unrealistic. Several suggestions haven been proposed by the researchers to address the above problem. The first attempt to mitigate the mass conservation problem of the level set method was executed by Sussman,1994, [4] using the iterative Re-initialization procedure of the level set equation which governs the motion of the dynamic interface. Although this approach was capable of reducing the mass loss or gain problem to a great extent still some significant amount of error was there in their solution. Later Chang et. al,1995, [5] introduced a new approach consisting of a new re-initialization equation for mass conservation which resembles the perturbed Hamilton-Jacobi equation in addition to the re-initialization of the level set function. This method involves complex mathematical calculations and is also difficult to understand physically. However, in [6], [26], [31] the main focus was placed on the Level Set Re-distancing Method to get accurate mass conservation during numerical simulation of incompressible two-phase flow problems. In the Level set Re- distancing Method, the re-initialization procedure of the level set function was modified by imposing a new constraint as a corrective measure of the mass loss problem. Yap et.al in the year 2007, [16] introduced a Finite volume-based Global mass conservation scheme to overcome the mass loss problem of the level-set method where CLAM schemes were used to model the convection of the level- set equations.

Apart from the approaches as mentioned above, few conservative approaches are there in literature to ensure mass conservation of the level set method. In [14] Olsson modified the standard level set method by introducing a new conservative scheme to discretize the level set advection equation and used an intermediate step

to keep the shape and thickness of interface constant which results in good conservation of area (volume in case 3D) occupied by the interface. Despite good mass conservation, the above method suffers from a slow convergence rate problem. In [15] corrective measures for the above problem were taken by considering diffusion only normal to the interface and also adaptive mesh control technique was included to find accurate information near the interface using grid refinement. The conservative methods proposed by Olsson et.al [14,15] was not based on any physical basis, so exact mass conservativeness may not be possible always from the above methods. This problem was resolved by Majumder and Chakraborty in 2005 [13] by introducing a physically based mass conservative Level set method for incompressible two-phase flows where the Heaviside function was replaced by volume-fraction based function to ensure the accurate mass conservation of individual phase present in the actual physical problem. Although the above method provides a good understanding of numerical simulation because of its simplicity but it suffers from local mass conservation problems and most importantly this method was not tested to handle three- dimensional multi-phase problem. However, in 2016, Mahmoudi et.al., [23] developed a novel conservative level set method to overcome the problem regarding mass conservation of the standard level set method, where the hyperbolic tangent function is used as a level set function, High order compact (HOC) difference scheme is used to transport the level set function and combined conservative difference scheme (CCD) is used to re-initialize the level set function.

Mass conservation in the standard level set method can also be achieved using the combined level set and volume of fluid method (CLSVOF) or the Combined Volume of Fluid and Level set method (VOFSET). Bourlioux [5] was the first one to introduce the coupled Level Set (LS) and Volume of fluid (VOF) known as the CLSVOF method where they developed the combination of these two superior methods to overcome the problem associated with mass conservation in the numerical simulation of incompressible two-phase flow. This Combined method utilized the advantages of both methods. In subsequent times, Sussman and Puckett [8] established a Coupled Level Set and Volume of Fluid (CLSVOF) for numerical simulation of 3D axisymmetric incompressible two-phase flows involving a large density ratio (1000:1). By seeing the great advantages of the CLSVOF method, Son and Hur [11] also initiated a new CLSVOF method for numerical simulation of buoyancy-driven flow. It is very important to note that all of the above-coupled methods proposed by eminent researchers are limited to first-order accuracy. The problem related to the accuracy of the aforementioned CLSVOF methods was mitigated by the development of a Second-order accurate Coupled Level set and Volume of Fluid (CLSVOF) method [12]. In recent times, dam-break flow-induced wave problems have been numerically investigated by Y.L.Li et al [29], using an improved version of the CLSVOF method where the Tangent of Hyperbola for Interface capturing/Weighted Line Interface Calculation (THINC/WLIC) Scheme is taken for accurate interface representation and ensuring excellent mass conservation. Apart from the CLSVOF method, the Coupled Volume of Fluid and Level Set (VOFSET) method proposed by Sun and Tao in 2010 [18] has drawn a lot of attention from computational scientists because of its simplicity and is numerically inexpensive.

In the VOFSET Method, the interface is advected by the Volume of fluid (VOF) method, and the level set (LS) function near the interface is calculated from an iterative geometric approach which is utilized to calculate the accurate interface curvature and smoothens the discontinuous physical properties across the interface. Recently Cao et al [27] have introduced an improved version of the VOFSET method for the numerical simulation of incompressible two-phase flow using unstructured quadrilateral grids in irregular domains. The analytic piece- wise linear interface calculation (PLIC) method is included here to enhance the speed of numerical computation.

In contrast to the above level set methods, Enright et al in 2002 [10] first developed a hybrid particle level set (PLS) method, where Lagrangian markers were used to correct the front location predicted by the Eulerian approach for ensuring accurate mass conservation in the standard level set formulation of incompressible two-phase flow problems. Based on this PLS method a wide range of practical problems, including rotation of Zalesak's disk, deformation of circular bubbles, and deformation of rotation field involving a moving interface were numerically simulated. The major drawback of the PLS method proposed by Enright is the misplacement of newly seeded particles in the opposite signed domain which as a result degrades the performance of the corresponding method. This problem was overcome by Archer and Bai in 2015 [20] by using a non- overlapping concept, which judges the suitability of potential new particles based on the information contained within the

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particle representation of the interface. Liang et al,2015, [21] got some satisfactory results from the numerical simulation of multi-phase flow problems using an optimized particle level set method. For optimization of the computational efficiency of the original PLS method introduced by Enright [10], Lanhao et.al in 2018 [28] had developed a new method known as One Layer Particle Level Set method (OPLS) where Lagrangian particle-based correction procedure is performed after the Level Set advection and re-distancing steps.

Now in this paper, Single bubble rising problem in a matrix involving large density ratio (i.e. 1000) with and without considering surface have been numerically investigated using the physically possible mass conservative level set method of COMSOL multi-physics software version 6.2. However, transient evolution of a single bubble in a horizontal developing flow field has also been taken to illustrate the robustness of this proposed numerical method. In these all case studies excellent mass conservation of individual fluid phase has been reported by using the proposed mass conservative level set method. Few bench mark incompressible two-phase flow problems in a rectangular geometry which includes merging of two-bubble having same density in a matrix with and without considering surface tension and rising of a single bubble involving different density ratio, viscosity ratio and also different magnitude of surface tension have been numerically solved for the purpose of proposed model validation.

Mathematical Modelling
2.1 Governing Equations
The governing equations for unsteady multiphase flow problems are the continuity and the incompressible Navier-stokes equation. Now the governing equations for individual fluid phases are given below:

For fluid-1
Continuity equation;
As the individual fluid phase is assumed as incompressible so the velocity field is divergence free and the continuity equation becomes as follows.
$$\nabla \cdot u_1 = 0 \qquad (1)$$
Where $u1$ is the velocity field of the fluid-1 region.
Momentum equation;
$$\rho_1 \frac{Du_1}{Dt} = -\nabla P_1 + 2\mu_1 \nabla D + \rho_1 g \,, \quad x \in fluid\ 1 \qquad (2)$$

For fluid-2;
Continuity equation;
$$\nabla \cdot u_2 = 0 \qquad (3)$$

Momentum equation;
$$\rho_2 \frac{Du_2}{Dt} = -\nabla P_2 + 2\mu_2 \nabla D + \rho_2 g \,, \quad x \in fluid\ 2 \qquad (4)$$

Where $\mathcal{D}$ is the deformation rate tensor and its components are defined as
$$D = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_i}\right],$$

g is the acceleration due to gravity,
ρ and μ are the density and Viscosity of the fluids respectively and it is important to note that these density and viscosity are different for different fluid phases. $\frac{D}{Dt}$ present in the above mathematical equations is known as material derivative and the subscripts 1 and 2 denote the fluid region 1 and 2 respectively.

Effect of surface tension present at the interface between two-distinct phases is to balance the normal stress across the interface Γ and creates the interface boundary condition. Now, the interface boundary condition [32,33] is given as follows;
$$2\,\hat{n}(\mu_1 \mathcal{D} - \mu_2 \mathcal{D}) = (P1 - P2 + \sigma\kappa)\hat{n} \qquad (5)$$

And $u_1 = u_2$, $x \in \Gamma_d$

Where $\hat{n}$ is the outward drawn unit normal vector to the interface which is defined by Γ and P_1, P_2 are the pressure at the interface on fluid 1 and fluid2 side respectively. σ is the coefficient of surface tension and κ is the curvature to the interface between two distinct phases. The domain containing two - distinct fluid phases is denoted as Ω and its boundary is denoted by $\partial\Omega$. Since, there is no penetration of fluid flow across the boundaries of the flow domain so we have the following boundary condition given below.

$$\boldsymbol{u.n} = 0 \text{ on } \partial\Omega. \qquad (6)$$

Level Set Formulation

The Level set method is a Eulerian computational approach for capturing the moving interface, which is a very famous method especially in the field of incompressible multi-phase flow problems. There are three functions in this novel method;

- Level set function to represent the interface between two distinct phases.
- Heaviside function to calculate any physical properties within the flow domain.
- Dirac delta function to model surface tension concentrated on the interface as a source term in the momentum equation.

Level set Function

The fundamental concept of interface representation using the level set function is based on the concept of implicit surfaces. Level set function is denoted by ϕ and it is defined at every point within the flow domain and have a fixed value at the interface. Level set function is the scalar function defined as
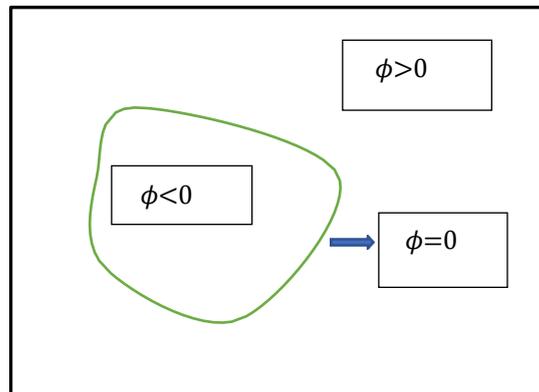
Fig-1; Interface representation using level set function

signed normal distance function measured from the pertinent location of the interface between two distinct phases. The absolute value of the level set function, ϕ at any point within the flow domain is defined as the normal distance of this point from the pertinent location of the interface.

It is assumed that if the point is taken inside the interface, ϕ is assigned negative value whereas it is assigned positive value when the point is lying outside the interface and the points lying on the interface having the value of ϕ equal to zero. Thus, the interface Γ at any instant of time can easily be represented by the zero-level set of ϕ without any disturbance encountered during interface re- construction. Now the fluid region lies inside the interface is represented as fluid region-1 and the fluid lies outside the interface as region-2. The interface between two-distinct phases is driven by the existing velocity field u present in the flow domain. Velocity field for the individual fluid phase is defined based on the sign of ϕ as shown below;

$$\boldsymbol{u} = \boldsymbol{u1} \text{ when } \phi < 0$$

$$\boldsymbol{u2} \text{ when } \phi > 0$$

In order to capture the dynamic evaluation of the moving interface, we have to compute the evolution of the points corresponding to ϕ=0 with respect to time.

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Now the governing equation for the dynamic evolution of the moving interface is given as follows;

$$\frac{\partial \phi}{\partial t} + u. \nabla \phi = 0 \qquad (7)$$

The equation (7) moves the interface (i.e. $\phi = 0$) based on the existing velocity field u accurately even in case of merging and breaking of bubbles. However, position of the interface at different instant of times can be computed by solving the above equation to the corresponding time step.

Now the outward drawn unit normal vector to the interface $\hat{n}$ and local curvature of the interface $\kappa(\phi)$ in terms of level set function ϕ is defined as follows;

Outward drawn unit normal vector, $\hat{n} = \nabla \Phi / |\nabla \phi|$

local curvature of the interface, κ is given as follows;

$$\kappa(\phi) = \nabla. \hat{n} = \nabla. \left(\frac{\nabla \Phi}{|\nabla \phi|}\right)$$

$$= \frac{\phi^2_{y} \phi_{xx} - 2\phi_{x} \phi_{y} \phi_{xy} + \phi^2_{x} \phi_{yy}}{(\phi^2_{x} + \phi^2_{y})^{\frac{3}{2}}}$$

The governing equation for flow field u along with interface boundary condition can be written as a single equation [6] as shown below.

$$\rho(\phi) \frac{Du}{Dt} = -\nabla p + \nabla. (2\mu(\phi)\mathcal{D}) - \sigma\kappa(\phi)\delta(\phi)\nabla\phi + \rho(\phi)g \qquad (8)$$

In the above equation, $\delta(\phi)$ is the Dirac delta function used to incorporate the surface tension concentrated at the interface between two-distinct phases into the momentum equation as a source term based on continuum surface force (CSF) model as described by Brackbill [32]. ρ, μ are the constant density and viscosity of the individual fluid phase and these properties being different for different fluid regions exist in the actual physical problem. That's why calculation of any physical properties like density, viscosity etc. at any point within the flow domain requires good choice of Heaviside function. The Heaviside function is a unit step function and its value depend on the sign of ϕ.

Now the density and viscosity at any point within the flow domain is given as follows;

$$\rho(\phi) = \rho_1 + (\rho_2 - \rho_1)H(\phi) \qquad (9a)$$
$$\mu(\phi) = \mu_1 + (\mu_2 - \mu_1)H(\phi) \qquad (9b)$$

Where H (ϕ) *is the Heaviside function* and its value according to the sign of the level set function ϕ is defined as [4].

$$H(\phi) = \begin{cases} 0 & \phi<0 \\ 0.5 & \phi=0 \\ 1 & \phi>0 \end{cases} \qquad (10)$$

This representation of the Heaviside function is also known as sharp representation because it causes sharp change of physical properties across the interface which in result creates numerical instabilities during numerical simulation of actual physical problem using the level set method [4,6]. Now to mitigate the numerical instability induced in the level set method due to the usage of the above sharp Heaviside function, a smooth

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Heaviside function is required for continuous variation of any physical properties like density, viscosity etc. across the interface.

The smooth Heaviside function as described in [4,6] is given below;

$$H_\varepsilon(\emptyset) = \begin{cases} 0 & if\ \emptyset < -\epsilon \\ \frac{\emptyset+\epsilon}{2\epsilon} + \frac{1}{2\pi}\sin(\pi\emptyset|\epsilon) & if\ |\emptyset| < \epsilon \\ 1 & if\ \emptyset > \epsilon \end{cases} \tag{11}$$

Now this equation shows that the interface between two-distinct phases is diffused and having finite thickness 2ϵ across which the Heaviside function is smoothed and resulting in continuous variation of physical properties of the individual fluid phase across the interface, thus avoiding numerical instabilities during mathematical modeling of the actual physical problem. However, it is important to note that the interface thickness is defined normal to the interface ($\phi = 0$) within the region $-\epsilon < \phi < \epsilon$ where ϵ is considered as factor of grid size. From the work of Sussman et.al [4] a correlation between finite interface thickness and grid size is taken and i.e. $2\epsilon = 3\Delta x$ where Δx is the grid size. From this correlation it can be easily concluded that with grid refinement the interface thickness will be reduced to a great extent and we can move toward the mathematical modeling of sharp interface without any numerical instability. Now, it should also be noted that $\phi = 0$ is the physically relevant interface and the value of the level set function (ϕ) within the diffused interface is numerically relevant because it is used to smooth the properties across the interface to avoid numerical instability. So, the value of the level set function outside the diffused interface have nothing to do in the numerical simulation of multi-phase flow problems.

Fig-2a shows the diffused interface where interface is represented by circular shape ($\phi = 0$) and having finite thickness of 0.8 unit. Representation of smooth the Heaviside function based on the sign of the level set function is shown below in fig-2b. Smooth Heaviside function within the diffused interface has two parts, the first part (i.e. linear part) has sudden change in slope at the ends of the interface whereas the second part (i.e. the sinusoidal part) varies smoothly. The addition of the sinusoidal part with the linear part of the Heaviside function makes its smooth variation across the diffused interface as shown in fig-2b.

Dirac delta function $\delta(\phi)$ in the equation (7) is used to model the surface tension concentrated on the interface as a source term into the momentum equation must be computed carefully because it is non-zero only on the interface and thus creates discontinuity across the interface, resulting numerical instability during mathematical modeling of multi-phase flow problems using level set method. As described in [34], the Dirac delta function $\delta(\phi)$ can be evaluated from the Heaviside function $H(\phi)$ during the Level set formulation of multi-phase flow problems as;

$$\delta(\emptyset) = \frac{dH(\emptyset)}{d\emptyset} \tag{12}$$

Now, in order to avoid the numerical instability due to this sharp Dirac delta function as described in the equation (12), smoothing of $\delta(\phi)$ is required similar to H(ϕ) as shown in equation (11). From [4] the smooth Dirac delta function can be defined as;

$$\partial\varepsilon(\emptyset) = \begin{cases} \frac{1}{2\varepsilon} + \frac{1}{2\varepsilon}\cos\left(\frac{\pi\emptyset}{\varepsilon}\right) & if\ |\emptyset| < \varepsilon \\ 0 & otherwise \end{cases} \tag{13}$$

Fig-2c shows the variation of smooth Dirac delta function across the diffused interface of thickness 2ϵ, where the $\delta s(\phi)$ decreases smoothly about $\phi = 0$ across the interface.

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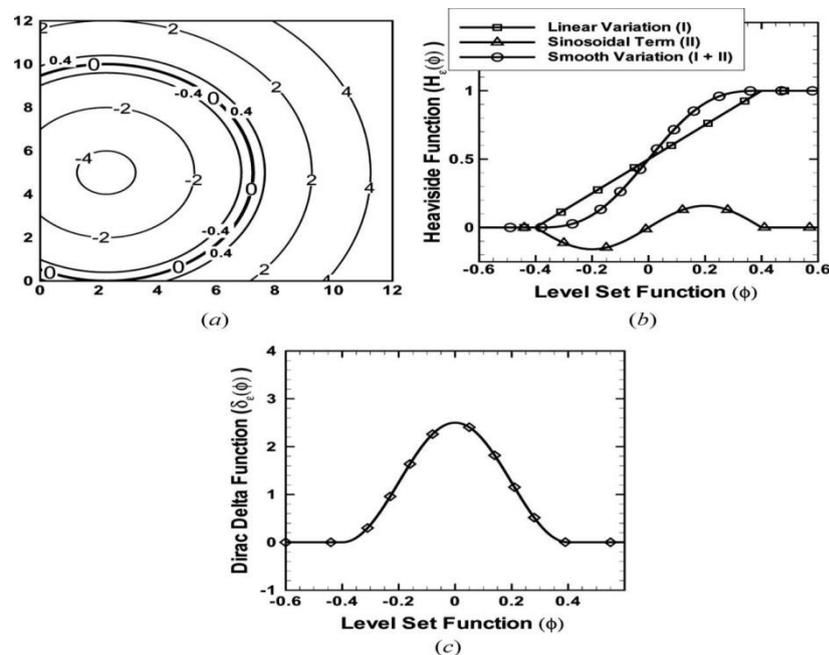
Fig-2; Smoothing in level set method. (a) Representation of diffused interface as a concentric circles (b) Representation of smooth Heaviside function (c) representation of smooth dirac delta function.

Re-initialization procedure;

From the above discussion, it is seen that to overcome numerical instability because of sharp changes of physical properties across the interface during numerical simulation of multi-phase flow problems using the level set method, the Heaviside function and the Dirac delta function must be smoothed over a finite thickness of the interface (i.e. 2ϵ). So, the mathematical modeling should be implemented in such a way that the required thickness of the interface will be independent of time. The thickness of the interface will be independent of time if the level set function acts as the signed distance function during the time domain of our interest. Although the level set function (ϕ) is initially defined as signed normal distance function from the pertinent location of the interface but it will not remain so after few iterations because of numerical diffusion. The problem of maintaining level set function as signed distance function was first resolved by Mark Sussman in1994 [4] by introducing re-initialization procedure. In this re- initialization procedure [4], an irregular level set function (ϕ) is re- initialized to signed normal distance function (ψ) by solving the following partial differential equation (PDE) under steady state condition.

$$\frac{\partial \varphi}{\partial \tau} = S(\emptyset)(1 - |\nabla\varphi|) \qquad (14)$$

$$and \quad |\nabla\varphi| = \overline{\sqrt{(\partial\varphi|\partial x)^2 + (\partial\varphi|\partial y)^2}}$$

Subjected to the following initial condition;

$\psi(\boldsymbol{x}, 0) = \phi(\boldsymbol{x}, t + \Delta t)$

Where, τ is the pseudo time and S is the sign function. For the ease of numerical simulation, the sign function is smoothed as follows [4].

$S_\in = \frac{\phi}{\sqrt{\phi^2 + \in^2}}$ where, $S_\in$ is the smooth sign function.

It is essential to note that during the re-initialization procedure, the location of the interface obtained after solving the advection equation (7) is not changed. From Fig. 3a and Fig. 3b, it has been observed that the location of zero-level set (i.e. the interface location) is not changed during re-initialization procedure. From equation (14), it is clear that the pseudo steady state solution of the same is the required signed distance function as it satisfies the advection equation (7). The initial condition of ψ ensures that the interface value of the same is equal to the value of ϕ at the interface. That's why the values of ψ obtained from the pseudo- steady state condition of the equation (14) are the values of the ϕ for t+Δt time step. Thus, by following the above re-initialization procedure, the level set function can easily be maintained as a distance function which is essential for accurate numerical simulation of multi-phase flow problems using the level set method. Now, the following condition is an essential criterion for the level set function to be a signed distance function from the interface location.

$$|\nabla \phi| = 1 \qquad (15)$$
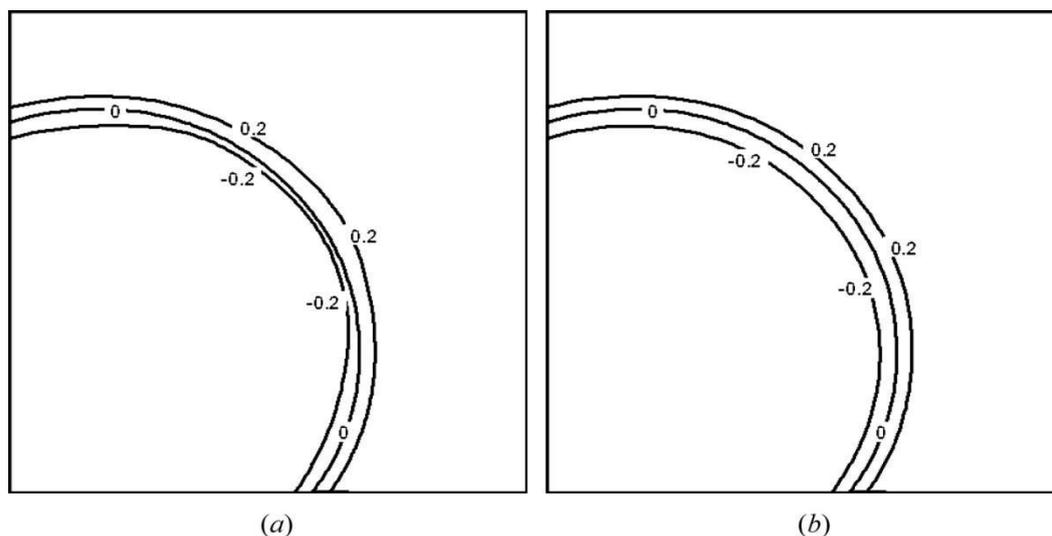
Fig. 3; Diffused interface (a) after advection (b) after re-initialization

Representation of mathematical model inside COMSOL

In this paper, applications of the mass conservative level set method in rectangular geometries are executed using COMSOL multi-physics software version 6.2. That's why, it is important to know the scenario taking place inside this CFD software while solving the incompressible two-phase flow problems in rectangular geometries using the mass-conservative level set method. In COMSOL multi-physics, the interface between two different phases is represented by 0.5 level set of ϕ, where ϕ varies smoothly from 0 to 1. For one fluid domain it is equal to zero and one for other fluid domain. Now, whatever governing equations are described above for general description of the mass conservative level set method, the same set of equations are also solved in this CFD software but there is a major difference, which lies on description of the moving the interface.

For accurate mathematical modeling of the moving interface without any numerical diffusion, the following equation is solved in COMSOL two-phase level set module.

$$\frac{\partial \theta}{\partial t} + u.v\phi = \gamma \nabla. (\varepsilon \nabla \phi - \phi(1-\phi).\frac{\nabla \phi}{|\nabla \phi|}) \qquad (16)$$

Where, u is the velocity of the existing flow field. Left hand side of the above equation gives the accurate motion of the moving interface whereas the right- hand part provides the numerical stability of the interface. The parameter

ϵ represents the thickness of the interface within which the level set function ϕ varies smoothly from 0 to 1. If the value of this parameter is too small or too large then numerical simulation will provide inaccurate results regarding the interface capturing and mass conservation. That's why optimization of ϵ is an essential requirement to capture the moving interface accurately. In COMSOL, the optimum value ϵ is set as half of the

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maximum element size ($hmax$) within the flow domain. However, another parameter γ determines the re-initialization or stabilization of the level set function and its value is changing based on the nature of the problems. The value of γ is playing a very critical role during mathematical simulation of moving interface, if its value is too small then oscillations in ϕ taking place due to numerical diffusion and as a result the thickness of the interface is not maintained as constant whereas if its value is too large then the interface moves inaccurately. That's why optimization of γ is also an essential criterion for capturing the interface accurately during numerical simulation of multi-phase flow problems especially while using the COMSOL multi-physics software. Therefore, in COMSOL the optimum value of the re-initialization parameter (γ) is taken as the expected maximum value of the velocity field present within the flow domain.

Representation of geometric properties of the interface like interface normal and local curvature of the interface in COMSOL is given as follows;

Outward drawn unit normal vector to the interface is:

$$\hat{n} = (\nabla\emptyset||\nabla\emptyset|)_{\emptyset=0.5}$$

Local curvature of the interface is:

$$k = -\nabla(\nabla\emptyset||\nabla\emptyset|)_{\emptyset=0.5}$$

$$= -\frac{\emptyset^2\emptyset_{y\ xx} - 2\emptyset_x \emptyset_y \emptyset_{xy} + \emptyset^2\emptyset_{x\ yy}}{(\emptyset_x^2 + \emptyset_y^2)^{\frac{3}{2}}}$$

Since, we are dealing with the incompressible multi-phase flow problems, so the velocity field is divergence free and it is defined as follows;

$$\nabla . \boldsymbol{u} = \boldsymbol{0}.$$

As the velocity field is divergence free, so the equation (16) can be written in the following conservative form.

$$\frac{\partial\emptyset}{\partial t} + \nabla . (u\emptyset) = \gamma\nabla . (\varepsilon\nabla\emptyset - \emptyset(1-\emptyset)\frac{\nabla\emptyset}{|\nabla\emptyset|}) \qquad (17)$$

This conservative form of the level set advection equation with re-initialization is helpful when exact numerical conservation is essential, especially for the exact area (or volume in 3D) conservation bounded by the interface when there is no inflow or outflow across the interface. By using the equation (17), accurate mass conservation of individual fluid phase is achieved during our numerical simulation of incompressible immiscible multi-phase flow problems with and without surface tension using two-phase level set module of COMSOL multi-physics software version 6.2, a Finite element method based CFD software.

During numerical simulation of time dependent multi-phase flow problems using mass conservative level set method of COMSOL multi-physics CFD software version 6.2, following equations are numerically computed inside this commercial CFD software.

Continuity equation; $\nabla . \boldsymbol{u} = 0.$

Momentum equation;

$$\rho(\emptyset)\frac{Du}{Dt} = -\nabla p + \nabla . (2\mu(\emptyset)D) + \sigma k(\emptyset)\emptyset\delta(\emptyset)\nabla\emptyset + \rho(\emptyset)g.$$

There is a slight difference between the momentum equation used in COMSOL as compared to that of the general description by equation (8). This occurs because of the difference in convention used during representation of the local curvature of the moving interface.

Level set advection equation with re-initialization;

$$\frac{\partial \emptyset}{\partial t} + \nabla.(u\emptyset) = \gamma\nabla.(\varepsilon\nabla\emptyset - \emptyset(1-\emptyset)\frac{\nabla\emptyset}{|\nabla\emptyset|})$$

Representation of level set advection equation which is also known as the governing equation for transport of moving interface is also quite different from that of the general description defined in the Equation (7). The reason is that in COMSOL re-initialization procedure for maintaining constant thickness of the moving interface is made integral to the level set advection equation by setting artificial time equal to real time whereas there is a separate representation of re- initialization procedure in general description as represented in equation (14).

"P1+p1" discretization technique is used to discretize the aforementioned continuity and momentum equation, where P1+p1 means both linear elements are used to solve the velocity and pressure field involving in the actual physical problem. However, "linear" discretization technique is used to discretize the level set advection equation with re-initialization while solving the multi-phase flow problem using the proposed mass conservative level set method of COMSOL Multiphysics version 6.2, a Finite element method (FEM) based CFD software.

Overall solution procedure using COMSOL multi-physics software version 6.2.

During numerical simulation of multi-phase flow problems using FEM based CFD software COMSOL, we have to follow the simple steps given below sequentially. Like any other CFD software, COMSOL has also three stages to solve any physical problem numerically and that are given below;

First; Pre-processing.
Second; Problem set up and computation.
Third; Post-processing.

First, we have to decide nature the problem (i.e. 2D or 3D) then accordingly selecting the type of geometry from model wizard section. After doing so we to have to add the physics of the problem going to be solved. Generally, based on suitable assumptions of the actual physical problem, we add the physics to the corresponding geometric model. Since we are dealing two-dimensional transient incompressible laminar two-phase flow problem, so we have added this physics to our suitable geometric model.

After completion of physics selection, the next step is the selection of nature of study (i.e. Stationary or time-dependent). By looking the actual physical problem, this study nature is considered. As mentioned earlier that we are dealing with unsteady two-phase flow problem, that's why we have added "time-dependent phase initialization" section in our numerical simulation.

After completion of the above-mentioned steps, a new window of this software will open. From this window we can setup the desired problem by providing valuable inputs like desired material properties, physically relevant boundary conditions, initial conditions and get the desired results upon successful completion of numerical computation. However, we can figure out valuable

insights from these results by proper utilizing the various post-processing tools available in this CFD software like other commercial CFD software has.

Results and Discussions
Model validation and Representative case studies;

The mathematical model used in this report is validated by comparing the results of the present method with the numerical results on merging of two bubbles with same density with and without consideration of the effect of surface tension by *Chang et. al* [6]. The problem geometry is shown in the fig. 4, where it is seen that the given problem is solved in a rectangular domain of non-dimensional size 1*1, non-dimensional radius of the upper bubble is 0.15 unit and its non- dimensional position is (0.5,0.65), non-dimensional radius of the lower bubble is

0.10 unit and its non-dimensional position is (0.5,0.35). Two-bubbles of same density are rising under the influence of gravity, the density ratio of the bubble and that of the surrounding medium is taken as 1:10. Viscosity of the fluid inside the bubble is 0.00025 unit whereas the viscosity of the surrounding medium is 0.0005 unit. It is important to note that in this problem the effect of surface tension is not considered. This problem is solved using free triangular mesh with maximum element size of 0.01 in COMSOL at different non-dimensional time steps i.e. t =0,0.1,0.2,0.3. As the bubble is lighter in weight than that of the surrounding medium, the bubble rises in the upward direction within the flow domain and results in different configurations of the moving interface at different time instances shown in the given fig. 5. The same problem has been numerically executed by *Chang.et.al* [6] at various time steps and their results are shown in fig. 6. Figures 5 and 6 show that the results obtained by the present method match excellently well with those obtained by *Chang.et.al.* [6], which validates the numerical method proposed in this report. The same problem has been numerically investigated with considering the effect of surface tension using the proposed method. In this case, surface tension is taken to be 0.005 and keeping all other parameters same. Fig. 7 shows the results of our numerical simulation using the proposed mass conservative level set method, whereas Fig. 8 shows the results of the same problem obtained by *Chang. et.al* [6]. Figures 7 and 8 show that the results obtained using the proposed numerical method match exactly with that of *Chang.et.al [6],* which also ensures the validity of our presented numerical method.
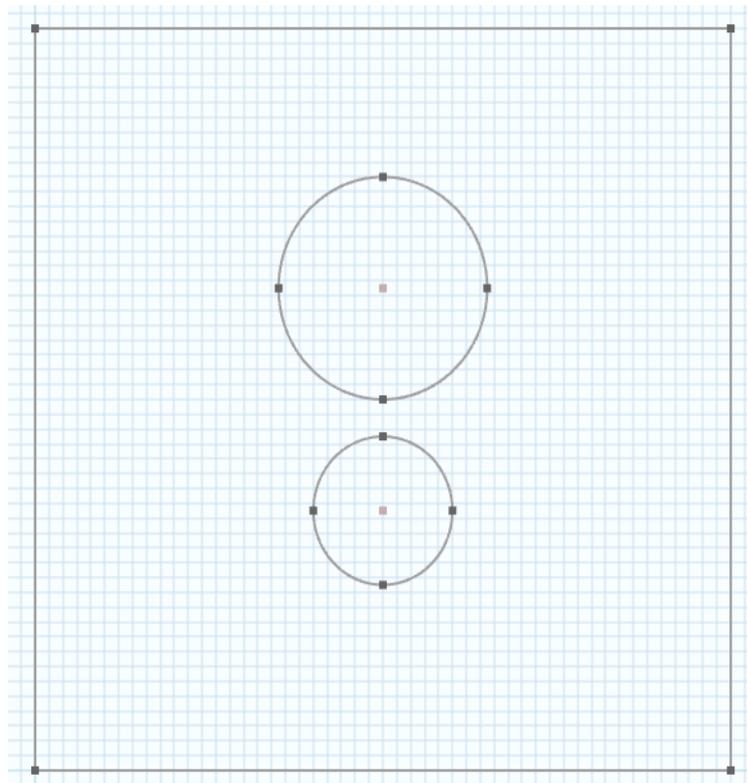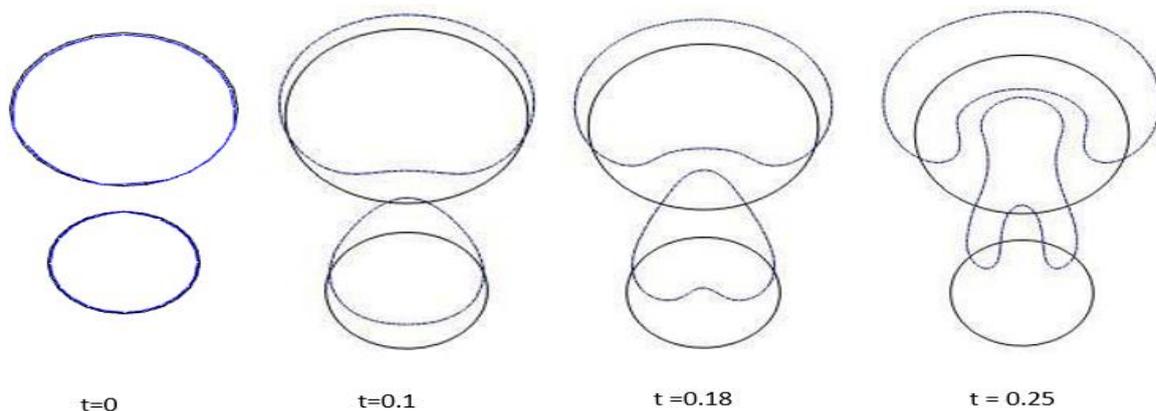

Fig. 4; Geometry of rising of two-bubbles problem.

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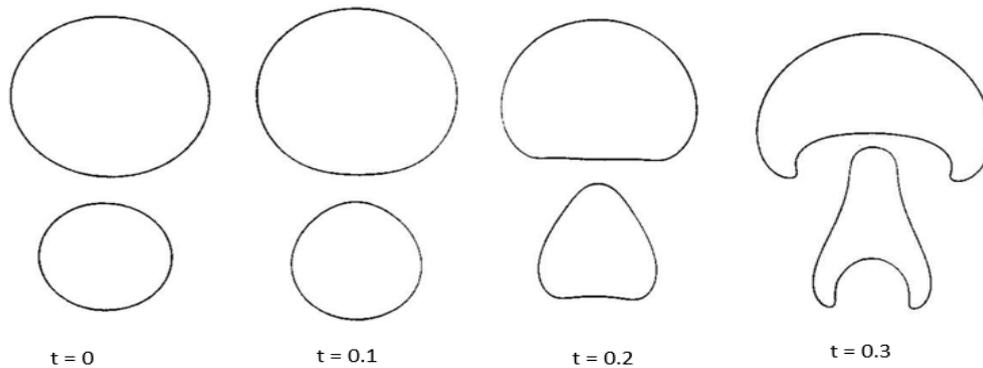t = 0   t = 0.1   t = 0.18   t = 0.25
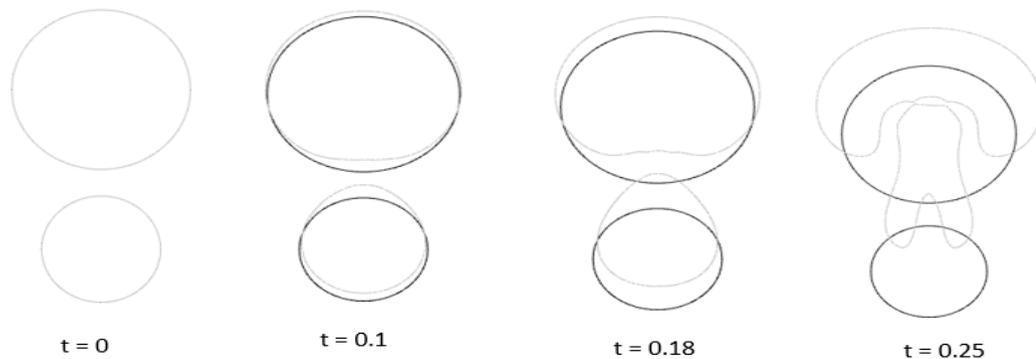
Fig. 5; Two bubbles of same density rising up. Density ratio between the bubbles and the background is 1:10, viscosity of the bubbles is 0.000 25 units and that of the background is 0.0005-unit,Surface tension .Free triangular mesh of maximum element size=0.01unit is used. Solution is obtained using COMSOL, a FEM based CFD software.

t = 0   t = 0.1   t = 0.2   t = 0.3
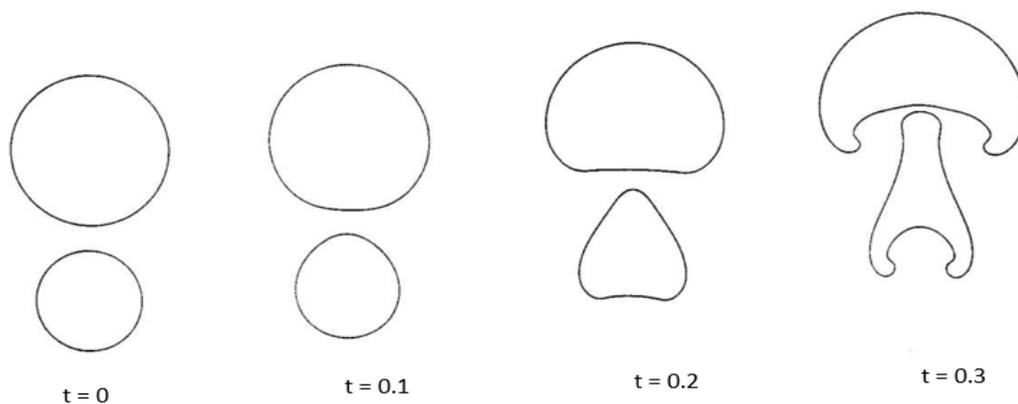
Fig. 6; Two bubbles of same density rising up. Density ratio between the bubbles and the background is 1:10, viscosity of the bubbles is 0.000 25 unit and that of the background is 0.0005 unit. This result was obtained by Chang et.al. using 256*256 grid size and there was no surface tension.


t=0   t=0.1   t =0.18   t = 0.25

Fig. 7; Two bubbles of same density rising up. Density ratio between the bubbles and the background is 1:10, viscosity of the bubbles is 0.000 25 unit and that of the background is 0.0005 unit. Surface tension of 0.005.

t = 0   t = 0.1   t = 0.2   t = 0.3

Fig. 8; Two bubbles of same density rising up. Density ratio between the bubbles and the background is 1:10, viscosity of the bubbles is 0.000 25 unit and that of the background is 0.0005-unit, Surface tension is 0.005. These results were obtained by *chang et.al.,*
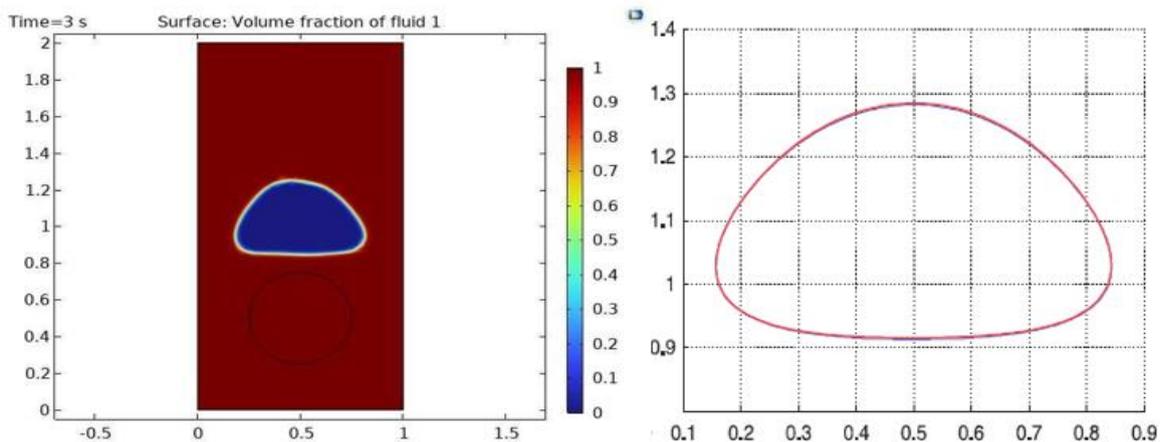
However, the proposed numerical method has been validated by comparing its results with respect to the numerical simulation results of a single bubble rising problem in two-dimensional rectangular geometry by *Hysing et.al.,* [36]. Initial configuration and boundary conditions of the single bubble rising problem under non-dimensional atmosphere are represented in the Fig.9. This problem was evaluated numerically under two test categories by *Hysing et.al.,* [36]. The parameters defining these two test cases are shown in table-1. Here, we have evaluated this problem using same set of problem data as that used by *Hysing et. al.,* [36]. The problem has been numerically simulated using unstructured quadrilateral mesh of grid size 0.0125 up to time t = 3. Fig.10(a) and Fig.10(b) depicts the numerical simulation result of the proposed method and result of *Hysing et. al.,* [36] respectively for the first test case at time, t = 3. These two figures show that result from the proposed mass conservative level set method matches excellently well with those by *Hysing et.al.,* [36]
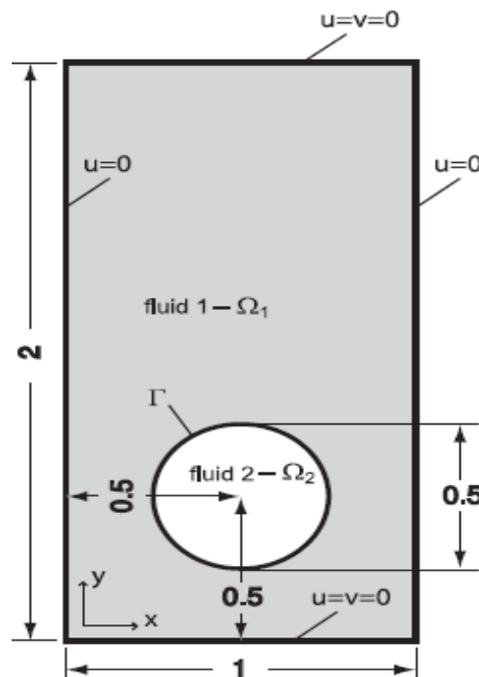
Fig. 9; Initial configuration along with boundary conditions for two test cases of single bubble rising problem.

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Table-1

Test case	$\rho 1$	$\rho 2$	$\mu 1$	$\mu 2$	σ	g
1	1000	100	10	1	24.5	0.98
2	1000	1	10	0.1	1.96	0.98

**Fig. 10; Bubble shape for first test case at t=3. (a) result of the proposed Numerical method. (b) result from the numerical computation by Hysing *et. al.*,**

In the second test case, bubble rising under large density ratio, viscosity ratio and small surface tension is numerically computed using our proposed method. Shapes of the bubble at different time instances computed by the proposed numerical method are shown in Fig.11. It is found that our results are in good agreement with those obtained by Hysing et.al., [36]. The results from the numerical computation by Hysing et. al., [36] are shown in the Fig.12. Now, it is also clearly visible that the original circular shape of the bubble is getting disturbed and break up takes place due to the smaller value of surface tension concentrated on the interface between two-distinct phases.

In these two test cases, results of our proposed method match excellently well with those by Hysing et. al., [36], which validates our proposed mass conservative level set to handle single bubble rising problem.
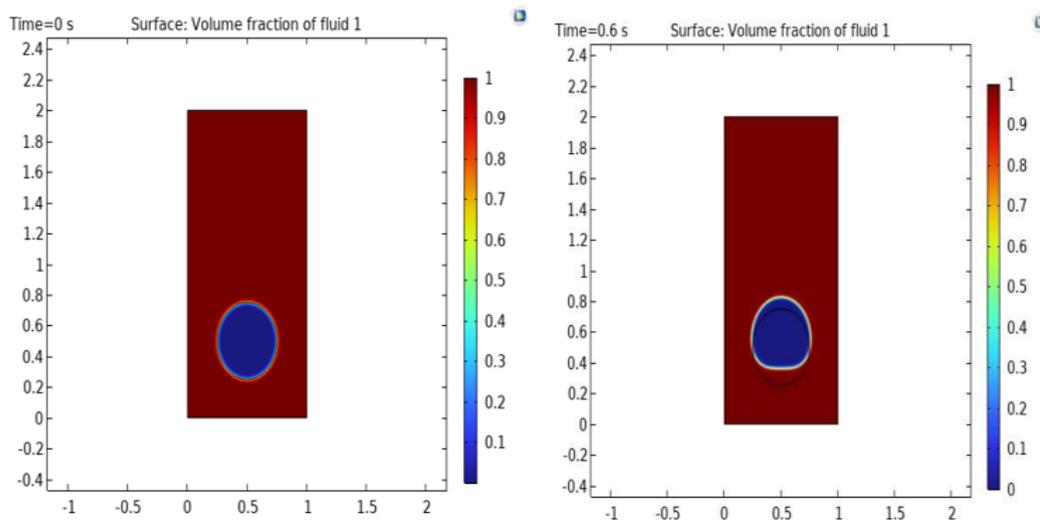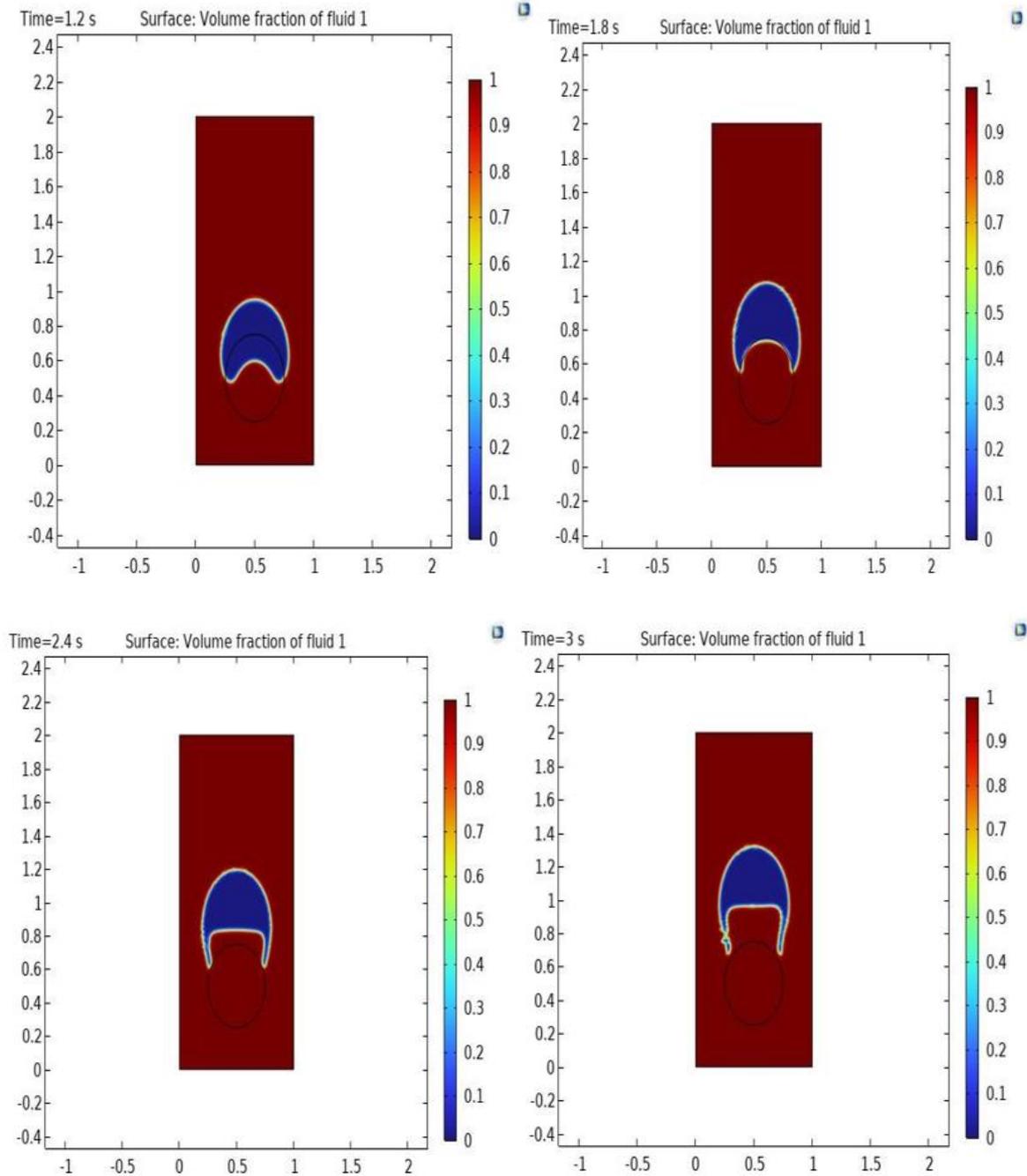
Fig. 11; Bubble configuration at different time instances for second test case using the proposed numerical method.
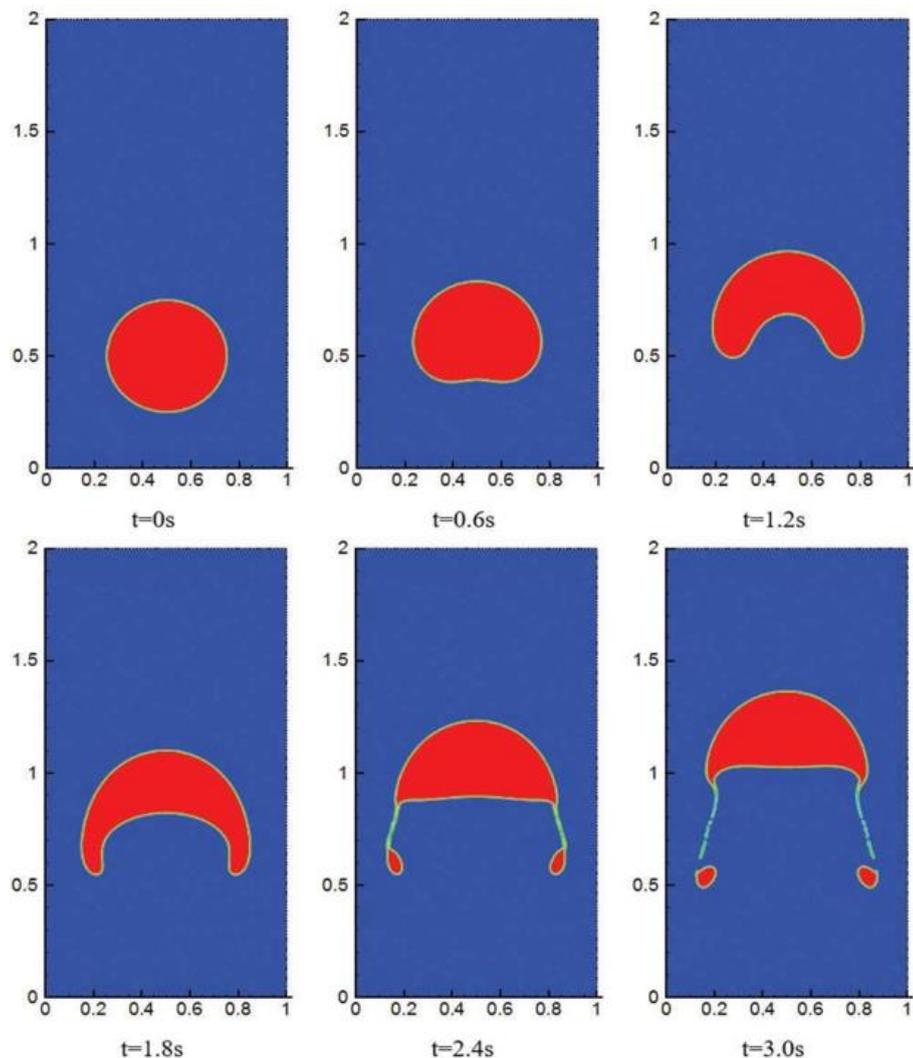
Fig.12;Bubble shapes at different time instances for second case study by *Hysinget.al.*,

Conclusion

A numerical study has been completed for the analysis of the two-phase flow using the level set method with physical possible conservation of mass. The present results have been validated using some benchmark problems considering grid independence study. A few case studies have numerically experimented considering with and without surface tension. It has been found that the rising bubble has been fragmented. The rising bubble fragmentation with no surface tension is dramatically different from with surface tension. With surface tension the bubble is more sturdy with respect to without surface tension. This means surface tension resists the fragmentation of the bubble which we have clearly shown in this analysis. Also, the popular notion that the shear force acts at angle of 45 and the cox angle is clearly observed in this analysis.

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