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THROUGH CFD SIMULATION**

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ABSTRACT

In nuclear systems the sub-cooled boiling flow is an important problem due to the behavior of condensing vapor bubble which has a large effect on the heat transfer characteristics as well as pressure drops and flow instability. The sub-cooled boiling flows become very complex and dynamic phenomena by the vapor bubble-water interaction. This happens due to the boiling / condensation, break-up, and coalescence of the bubble and needs to be addressed for characterizing the above mentioned flow parameters. There have been many researches to analyze the behavior of bubble experimentally and analytically. However, it is very difficult to get complete information about the behavior of bubble because of ever changing interface between vapor and water phase due to bubble condensation/ evaporation. Therefore, it is necessary to carry out a CFD simulation for better understanding the complex phenomenon of the bubble behavior. The present work focuses on the simulation of condensing bubble in subcooled boiling flow using (Volume of Fluid) VOF method in the CFD code CFD-ACE+. In order to simulate the heat and mass transfer through the bubble interface, CFD modeling for the bubble condensation was developed by modeling the source terms in the governing equations of VOF model using the User-Defined Function (UDF) in CFD-ACE+ code. The effect of condensation on bubble behavior was analyzed by comparing the behavior of condensing bubble with that of adiabatic bubble. It was observed that the behavior of condensing bubble was different from that of non condensing bubble in respect of bubble shape, diameter, velocity etc. The results obtained from the present simulation in terms of various parameters such as bubble velocity, interfacial area and bubble volume agreed well with the reported experimental results verified with FLUENT code in available literature. Hence, this CFD-ACE+ simulation of single bubble condensation will be a useful computational fluid dynamics tool for analyzing the behavior of the condensing bubble in a wide range of the sub-cooled boiling flow.

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1. INTRODUCTION

There are many industrial applications such as nuclear reactors, boiler etc. where systems are encountered with subcooled boiling flow regime. The knowledge of heat transfer in these systems under subcooled boiling where in condensing bubbles affect the pressure drop and instability is essential as this has a bearing on the design and the safety of the system. The change in bubble dynamics as a result of condensation makes it difficult to understand the subcooled boiling flow phenomenon, due to the interface heat and mass transfer. It is an impossible task to obtain complete information about the bubble behavior due to the existence of the bubble interface between the vapor and liquid phases. In addition to that, in subcooled boiling flow, bubble condensation significantly affects the change of interface so this complicates the analysis of the behavior of condensing bubbles even more.

The motion of bubbles is very complex. They may be subject to break-up or coalescence and may appear to move with a spiraling, zigzagging or rocking behavior. The phenomena, which are associated with fluids of high-density ratio i.e. 2000:1 and low viscosity, are not yet fully understood. In particular, the motion, the wake and the shape of bubbles are the subjects of active research. Again, bubble growth in subcooled flow involves top condensation when bubble emerges through subcooled bulk. Recently, many studies have been carried out to numerically simulate the rising bubble in various conditions. In those simulations, different parameters describing the behavior of the rising bubble were analyzed such as the bubble sizes, shapes, trajectory and velocity. One of the numerical methods for bubble simulation is the Volume of Fluid (VOF) model proposed by Hirt and Nichols^[1]. They dealt flow of immiscible fluids with a defined interface. R. Krishna and J. M. Van Bayten^[2] attempted to simulate the motion of single gas bubbles in a liquid using the VOF technique, which describes the complex bubble dynamics using only the fluid phase properties as inputs. R. Krishna and J. M. Van Bayten^[3] studied the rise characteristics of a rising bubbles in a 2D rectangular column and to solve the Navier-Stokes equations of motion, a commercial solver CFX 4.1 was used. They developed their own bubble-tracking algorithm to capture "sinuous" bubble motions. Afshin Ahmadi Nadooshan and Ebrahim Shirani^[4] used six different surface tension models for interfacial flows to simulate bubble rise and obtained results in close agreement with the experimental data. They concluded that the bubble shape remains spherical and smooth and compares with experimental result when it is small. All these studies confirmed that the VOF model can yield good predictions of the bubble shape and velocity. However, all the above studies were limited to adiabatic bubble where heat and mass transfer between the phases were not considered. In subcooled boiling flow, bubble condensation is the main feature which affects the shape and velocity of the bubble due to varying interfacial area.

Interfacial heat and mass transfer is the key consideration to understand the bubble behaviour in subcooled boiling flow.

In past many numerical studies have been performed to understand the heat and mass transfer through bubble interface. De-wen Yuan et al^[5] did a numerical investigation for a bubble growth process in sub cooled boiling flow. The process of bubble growth was realized by VOF model and User-Defined Function (UDF) interface through CFD software FLUENT. The simulation results well reflect bubble growth process as a dynamic result of evaporation and condensation which agree the experimental results very well and the relationship between the vapor-liquid interface motion and velocity field inside the bubble are also presented here.

A numerical study was carried out by Bernardo and Legendre^[6] for the mass and heat transfer from deformed bubbles rising in stationary viscous liquid. The numerical code JADIM that solves the Navier-Stokes equations, coupled with diffusion advection of a passive scalar was used to characterize the effect of the bubble deformation on the interfacial transfer. Different types of boundary fitted numerical grids were tested in order to obtain reliable results for the mass/heat transfer.

Seong et al^[7] focused on simulation of the bubble condensation in CFD code FLUENT through VOF approach. In order to simulate the heat and mass transfer through the bubble interface, CFD modeling for the bubble condensation was developed by modeling the source terms in the governing equations of VOF model using the User-Defined Function (UDF) in FLUENT code. For the validation of the UDF of bubble condensation, the results of the CFD simulation were compared with the results of a bubble condensation experiment performed in Seoul National University (SNU)^[8].

In the present work, an attempt was made to capture the behaviour of condensing bubble flowing in a channel ,by using commercial CFD code CFD-ACE+ through VOF model. A User-Defined Function was developed to simulate interfacial heat and mass transfer during condensation. The effect of condensation on bubble behavior was analyzed by comparing the behavior of condensing bubble with that of adiabatic bubble. It was observed that the behavior of condensing bubble was different from that of non condensing bubble in respect of bubble shape, diameter, velocity etc. For validation of CFD-ACE UDF of bubble condensation, an inter code comparison was made and it agreed well with the experimentally validated results from FLUENT code in available literature^[7]. Through this work an emphasis was put on VOF module along with the development of an UDF for bubble condensation in CFD-ACE+ code. This theoretical study is motivated by the future CFD application and the intent to investigate the capabilities of the CFD-ACE+ package.

2. Mathematical modeling

2.1 The VOF Module

In CFD-ACE+ engine, the Volume of Fluid (VOF) method is a numerical technique for tracking and locating the free surface (or fluid-fluid interface). It belongs to the class of Eulerian methods which are characterized by a mesh that is either stationary or is moving in a certain prescribed manner to accommodate the evolving shape of the interface. It is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest. The basis of the VOF interface tracking method was presented in 1980 by Hirt et al.^[1], but recently extended in 1995 by Rider et al.^[9]. Latest in 1996 Rider et al.^[10] have made great progress in including the surface tension effects in a more consistent manner. The VOF method used in CFD-ACE+^[11] is mainly based on these last two articles. In the VOF model, a single set of momentum equations is shared by the fluids, and the volume fraction (α) of each of the fluids in each computational cell is tracked throughout the domain. This method consists of three ingredients: a scheme to locate the surface, an algorithm to track the surface as a sharp interface moving through a computational grid, and a means of applying boundary conditions at the surface. In VOF model, the governing equations are solved using the volume fraction in each cell. In each cell, the summation of the each phase's volume fraction is unity.

For every grid cell, if

- $\alpha_i = 0$, the cell is empty of the i^{th} fluid
- $\alpha_i = 1$ when the cell is full of the i^{th} fluid.

The cell contains the interface between the i^{th} fluid and one or more other fluids when $0 < \alpha_i < 1$. For two-phase problems, the region $0 < \alpha_i < 1$ represents the interface region separation the two fluids. This condition can be used for interface tracking.

In VOF model, all properties are calculated using the volume fraction in each cell. In two-phase system, if the phases are represented by the subscripts 1 and 2, and if the volume fraction of the second phase is being tracked, the density (ρ) in each cell is determined as follows.

$$\rho = \alpha_2 \rho_2 + (1 - \alpha_2) \rho_1 \quad (1)$$

All other properties such as viscosity are computed in the same manner. Therefore, properties in each cell become different based on the volume fraction. And governing equations are solved using these properties. Here, the change of the bubble interface is tracked by the solution of a continuity equation for the volume fraction. For the i^{th} phase, this equation has the following form,

$$\frac{\partial \alpha_i}{\partial t} + \vec{u} \cdot \nabla \alpha_i = \frac{S_{\alpha_i}}{\rho_i} \quad (2)$$

Where, S_α is the mass source term. The mass transfer during the condensation of the vapor bubble can be controlled by modeling the mass source term as per the requirement. In VOF model, a single momentum equation is solved throughout the domain, and the obtained velocity field is shared among the phases.

$$\frac{\partial}{\partial t}(\rho \vec{u}) + \nabla(\rho \vec{u} \vec{u}) = -\nabla p + \nabla \left[\mu \left(\nabla \vec{u} + \overline{\nabla \vec{u}^T} \right) \right] + \rho \vec{g} + \vec{F} \quad (3)$$

Where, v is treated as the mass-averaged variable.

$$u = \frac{\sum_{i=1}^2 (\alpha \rho u)_i}{\rho} \quad (4)$$

In this bubble simulation, \vec{F} represents the volumetric forces at the interface resulting from the surface tension. The energy equation, shared among the phases, is shown below.

$$\frac{\partial}{\partial t}(\rho E) + \nabla(\vec{u}(\rho E + p)) = \nabla[k_{eff}(\nabla T)] + S_h \quad (5)$$

The VOF model treats energy, E , and temperature, T , as mass-averaged variables.

$$E = \frac{\sum_{i=1}^2 (\alpha \rho E)_i}{\sum_{i=1}^2 (\alpha \rho)_i} \quad (6)$$

Where, E for each phase is based on the specific heat of that phase and shared temperature. The source term, S_h is the heat source term. In order to simulate the heat transfer between the phases during the bubble condensation, modeling the heat source term is required. In the cell, where vapor fraction is zero or one, governing equations are solved for only corresponding phases i.e., for water and vapor phases. In the interface cell, that is when void fraction is between zero and one, governing equations are solved for mixture phase. Source terms are used only in governing equations of interface cell because the heat and mass transfer occurs on the interface during the condensation. The complex bubble dynamics can be studied using these governing equations.

2.2 Modeling UDF for Bubble Condensation

The in- built VOF model of the CFD-ACE+ code is capable for capturing adiabatic bubble behavior. But, for simulating the bubble condensation, the source terms in the governing equations

(2) and (5) should be modeled for interfacial mass and heat transfer. In this study the User Defined Function (UDF) of CFD-ACE+ is used to model the source terms. The UDF is a subroutine written in the Fortran Programming language and is based on the predefined CFD-ACE+ user access routines and functions. User subroutines are built as Dynamic Link Libraries (DLL files for Windows). The shared libraries are then linked with CFD-ACE+ Solver such that a two way communication between the solver and the user defined input is established. It is possible to define user's own initial and boundary conditions and source terms. Present UDF program is based on following described bubble condensation in subcooled boiling flow.

2.2.1 Modeling of interfacial Mass and heat transfer

Bubble condensation occurs by convective heat transfer mechanism due to the temperature difference between vapor and water phase. Bubble condenses under the influence of subcooled liquid and heat would be transferred from bubble to the subcooled liquid through the interfacial area. Heat transfer rate between two phases is given by

$$\dot{q} = h_{in} A (T_{sat} - T_l) = \dot{M} h_{fg} \quad (7)$$

where h_{in} is interfacial heat transfer coefficient, T_{sat} , T_l are vapor and liquid temperature, respectively, A is the bubble interfacial area between two phases which is an user access parameter in CFD-ACE+.

\dot{M} is the total mass transfer rate from vapor to liquid in ($\text{kg}/\text{m}^3\text{s}$) and h_{fg} is the latent heat of vaporization.

In this study, the interfacial heat transfer coefficient, h_{in} is calculated based on Kim's Condensation Correlation by substituting dimensionless numbers such as Re and Ja , which are obtained by analyzing the behavior of the bubble every time-step. The condensation correlation has the following form.

$$Nu = \frac{h_{in} D_b}{k_l} = 0.2575 Re^{0.7} Pr^{-0.4564} Ja^{-0.2043} \quad (8)$$

Re represents the bubble Reynolds number, which is calculated using

$$Re = \frac{\rho_l U_r D_b}{\mu_l} \quad (9)$$

where, ρ_l is the density of the liquid, U_r is the relative velocity of bubble inside the liquid, μ_l is the viscosity of liquid and D_b is the diameter of the bubble. In equation (9) bubble relative velocity can be defined as

$$U_r = \sqrt{U_x^2 + U_y^2 + (U_z - U_l)^2} \quad (10)$$

U_x , U_y and U_z are the bubble velocity component at x , y and z directions, respectively. U_l is the local liquid velocity. In this study, the bubble is defined as an aggregate composed of cells which have the volume fraction in the range of $0.5 \leq \alpha_g$. So, the bubble velocity component was calculated from the change of centre of mass for the bubble at each time step.

$$U_x = \frac{\nabla X_{cent}}{dt} \quad (11)$$

Center of mass (X_{cent}) for the bubble is defined as:

$$X_{cent} = \frac{\sum_j (\alpha_{g,j} \cdot \rho_g \cdot V_{g,j} \cdot x_{cm,j})}{\sum_j (\alpha_{g,j} \cdot \rho_g \cdot V_{g,j})} \quad (12)$$

Where, $\alpha_{g,j}$ is the volume fraction of j^{th} cell, $V_{g,j}$ is the volume of j^{th} cell, ρ_g is vapor density and $x_{cm,j}$ is the centre of mass of j^{th} cell.

Now, the bubble diameter D can be calculated by

$$D = 6 \times \frac{\text{Bubble volume}}{\text{Interfacial area}} \quad (13)$$

Where, volume of bubble and interfacial area are user access variables and can be directly extracted from CFD-ACE+ code.

Substituting (10) and (13) into (9) yields bubble Reynolds number.

Jacob number for the liquid, Ja is defined as

$$Ja = \frac{\rho_l \cdot C_{pl} (T_{sat} - T_l)}{\rho_g \cdot h_{fg}} \quad (14)$$

ρ_l is the density of liquid, ρ_g is the density of vapor, C_{pl} is the liquid specific heat, T_l is the local liquid temperature.

Prandtl number for the liquid, Pr is defined as

$$Pr = \frac{C_{pl} \cdot \mu_l}{k_l} \quad (15)$$

Where, k_l is the liquid thermal conductivity.

Interfacial heat transfer coefficient can be calculated by substituting (9), (14) and (15) into heat transfer correlation (8) and can be used to estimate the source terms.

The total mass transfer rate from vapor bubble to liquid is given by

$$\dot{M} = \frac{\dot{q}}{h_{fg}} = \frac{h_{in} A (T_{sat} - T_l)}{h_{fg}} \quad (16)$$

Because the total mass transfer rate is defined as the sum of each interfacial cell's mass transfer rate, the eqn. (16) can be re-written as

$$\dot{M} = \sum_j \alpha_{g,j} \dot{m} V_{in,j} \quad (17)$$

Where, $V_{in,j}$ is the volume of the j^{th} interface cell and \dot{m} is the average mass transfer rate i.e., the overall mass transfer rate divided by the total vapor volume in the bubble interface region. The mass source term in CFD-ACE+ is applied per cell as follows

$$S_{\alpha} = \dot{m} V_{in,j} = \frac{h_{in} \alpha_{g,j} (T_{sat} - T_{l,j}) A}{h_{fg} \sum_j \alpha_{g,j} V_{in,j}} V_{in,j} \quad (18)$$

Where $T_{l,j}$ is calculated as the local liquid temperature at the cell position in the interface.

The energy source term, in the j^{th} interface-cell is obtained by multiplying Eq.(18) by latent heat of vaporization.

$$S_h = \dot{m} h_{fg} V_{in,j} = h_{in} \frac{\alpha_{g,j} (T_{sat} - T_{l,j}) A}{\sum_j \alpha_{g,j} V_{in,j}} V_{in,j} \quad (19)$$

As the source terms are determined by local variables in Eq. (18) and (19), the local condensation rate in each interface-cell is different along the surface of the bubble. This UDF of bubble condensation simulates the condensing bubble with the CFD-ACE+ code. By applying (18) and (19), to the source terms in the interface cell, the amount of the bubble condensation can be calculated.

3. Test cases

It is good CFD practice to test the reliability of the solver/engine on simple test cases. In the present work, firstly, the CFD-ACE+ solver is tested on a 2D pure flow example where, an adiabatic bubble in subcooled flowing liquid in a rectangular channel was considered. The dynamical behavior of bubbles moving in a straight channel is used to investigate capabilities of the free surface VOF module. Secondly, to confirm the applicability of the developed CFD-ACE+ modelling into the VOF model, a single bubble condensation process has been simulated in subcooled flowing liquid in a rectangular channel.

4. Computation domain

The dimension of the 2D flow channel was 20 X 10 mm². The bubble diameter was 4 mm and was placed with its centre being 5 mm from the left edge and 3 mm from the bottom-edge. The flow direction was upward (positive Y-axis). The meshes of the flow channel were generated using structural meshing, quads-only of size 0.2 mm. Fig. 1 shows a schematic and computation grid of flow channel along with bubble

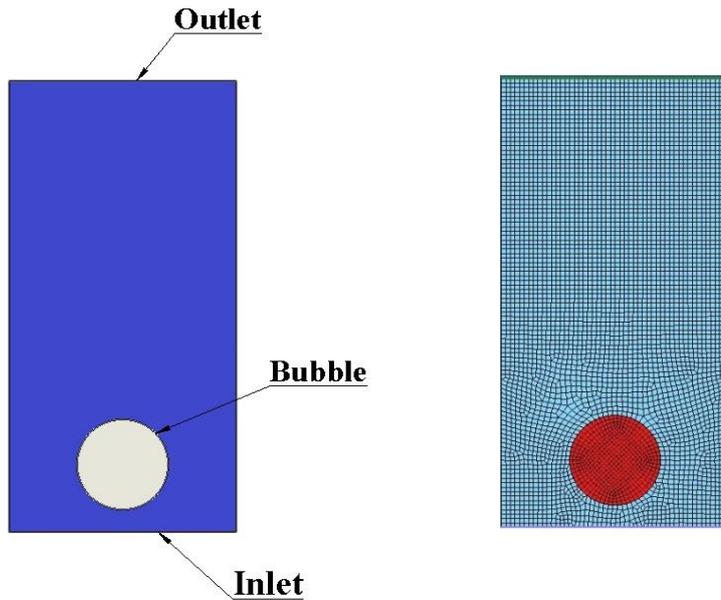


Figure 1 Schematic and computation grid of flow channel along with bubble

5. Boundary and Initial conditions

The developed CFD model is transient and thus, as an initial condition, all computations were started with a zero volume fraction for water and one for steam. Bubble growth process was neglected and it was assumed that a vapor bubble with a certain initial size (diameter) appeared in the flowing liquid just after the detachment from a heating surface. As boundary conditions, the inlet and outlet of the channel were modelled as velocity-inlet and pressure-outlet, respectively. All boundary walls were considered non-slip to the fluids. The inlet conditions such as the water velocity and the bubble temperature have been given constant as 0.1 m/sec and 373.2 K respectively. For the second test case, different water bulk temperatures were taken to understand the lifetime of condensing bubble at different level of subcooling. The surface tension is included by defining a constant value (0.072 N/m). Table 1 gives the overall view of test conditions.

Table 1 Test Condition

Case	Condensing Model	Liquid Temperature (K)	Bubble Temperature (K)	Liquid Velocity m/sec
1	Not applied	363	373.2	0.1 m/sec
2	Applied	363		
		353		
		343		

6. Numerical Scheme

The above test cases were simulated through VOF approach for investigating bubble behaviour i.e., bubble velocity and bubble diameter during adiabatic and condensation process. During all simulation cases in present work, a piecewise linear interface calculation (PLIC) interface reconstruction method has been used for interpolation in a cell. The first order up-wind differencing scheme is applied for the solution of momentum equation. The pressure-velocity coupling was obtained using the SIMPLEC algorithm which is recommended for usual transient calculations. Maximum allowed Courant number was set to 0.2. A Variable time step was used with the initial time step of 0.0001 sec and then varying between 0.00001 sec and 0.0005 sec. The solution converged in less than 10 iteration at each time step.

7. Results and Discussion

7.1 Model evaluation

The above test cases were simulated through VOF approach for investigating bubble behaviour i.e., bubble diameter during adiabatic and condensation process. The effects of condensation on bubble behaviour were analyzed by comparing the behaviour of condensing bubbles with that of adiabatic bubbles. Figure 2 shows the visual results for the behaviour of the non condensing vapor bubble. When the condensation modelling was not applied, just the shape of bubble was deformed as time goes by without the change of bubble size. When the condensation modelling was applied, the bubble was condensed as the bubble rose up. And from Fig. 3 to Fig. 5, it was found that the bubble condensed more rapidly due to addition of source term as the degree of subcooling increased. With the progression of time, the spherical shape of the adiabatic bubble is changed to a slightly ellipsoidal shape due to the influence of hydrodynamic force. The shape of the condensing bubble changes from spherical to ellipsoidal and then returns to the spherical shape as the condensation rate increases with the increase of degree of subcooling. With the increase of condensation rate, the bubble size became so small that the effect of surface tension is large enough to prevent a shape change.

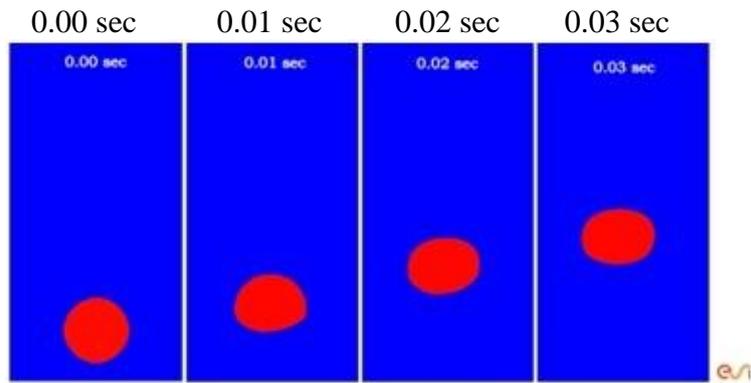


Figure 2 Visual presentation of Bubble behaviour with No Condensation

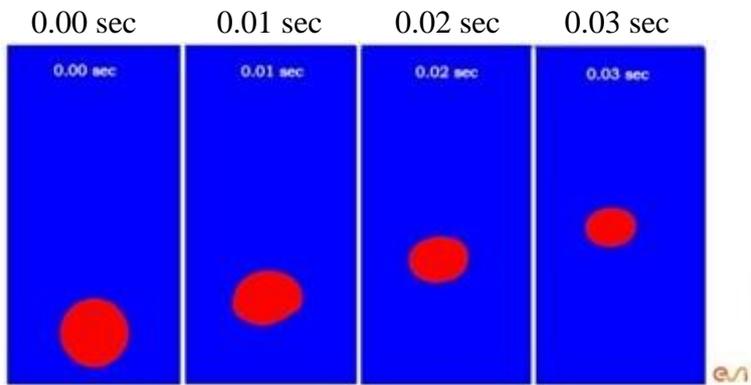


Figure-3 Visual presentation of Bubble behaviour with Condensation at 363 K

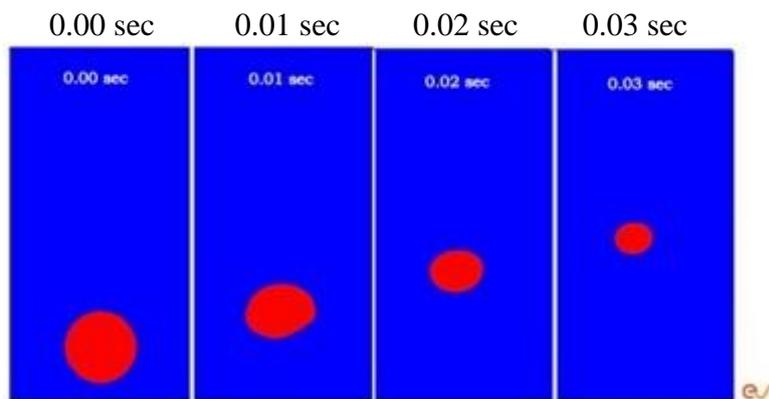


Figure-4 Visual presentation of Bubble behaviour with Condensation at 353 K

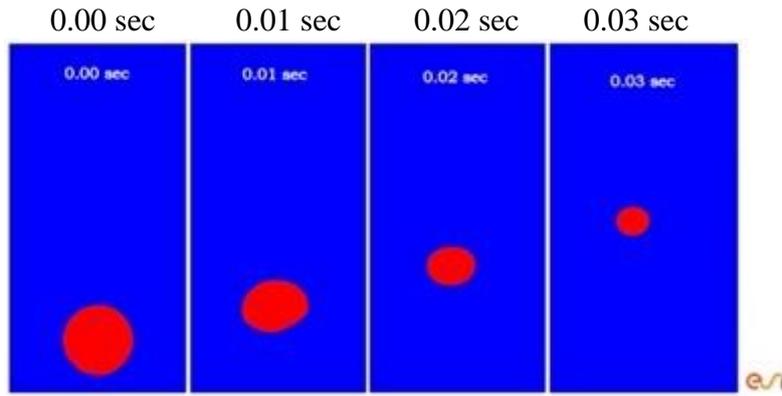


Figure-5 Visual presentation of Bubble behaviour with Condensation at 343 K

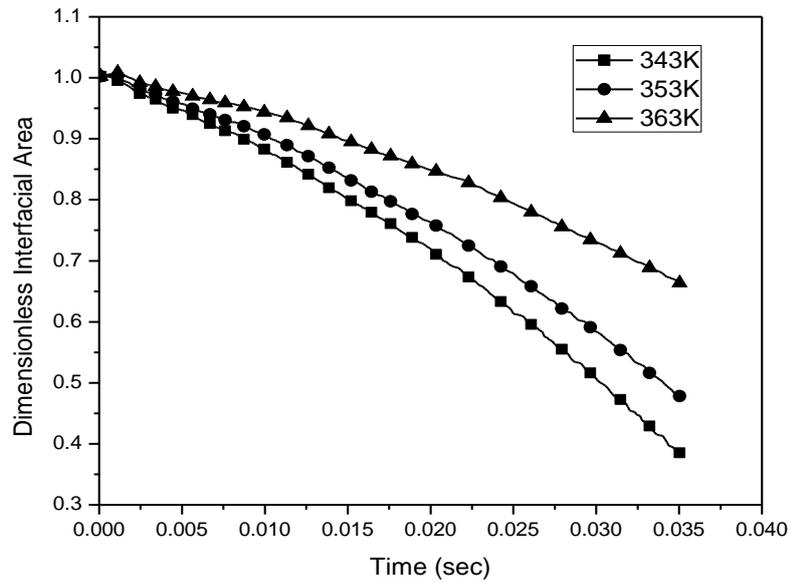


Figure-6 Interfacial area vs. time

Fig. 6 shows the variation of dimensionless interface area with time for different water temperatures. The dimensionless interface area, \bar{A} is calculated by

$$\bar{A} = \frac{\text{Instantaneous interface area}}{\text{Initial interface area}}$$

Fig. 7 shows the time-dependent bubble diameter. In case of adiabatic bubble, the diameter is constant. The bubble diameter decreases rapidly with the increase of degree of subcooling, the condensation rate increases as the mass transfer source term is directly proportional to the difference of the saturation temperature and the local liquid temperature.

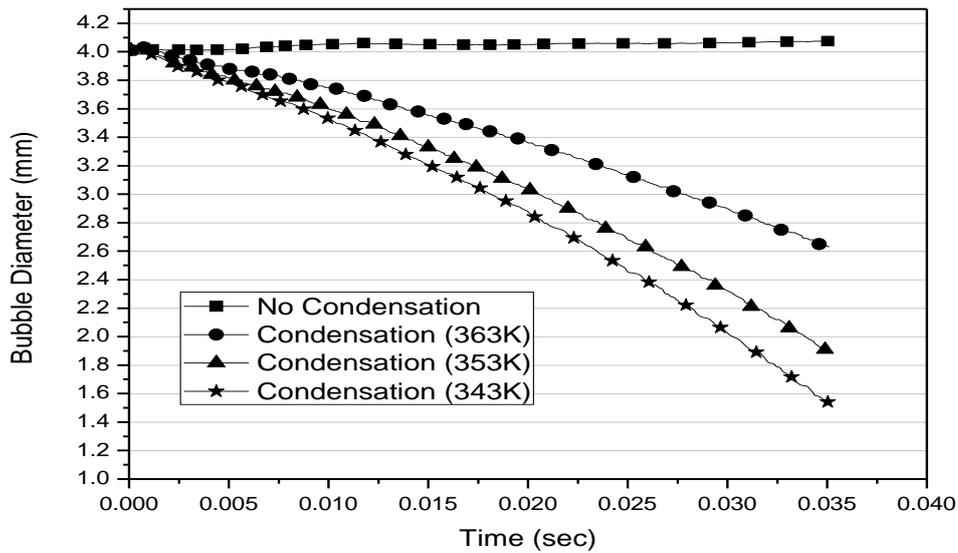


Figure-7 Bubble diameter vs. time

The simulation shows the time-dependent behavior of the bubble including features such as the bubble shape, size and interaction with the subcooled liquid. As time progresses, the vapor bubble rises up and is condensed in the subcooled flow. The asymmetric bubble shape is changed to an elliptical, irregular shape. From 2D simulations, it can be concluded that the VOF model coupled with the UDF of bubble condensation worked well and can be used to simulate behavior of the condensing bubble.

7.2 Validation

An inter code comparison was made for validation of CFD-ACE+ UDF of bubble condensation. The result obtained from the present work was compared with the experimentally validated results from FLUENT code in available literature [7]. Figure 8 shows the comparison of the CFD-ACE+ predicted and FLUENT predicted value for reduction of bubble diameter with time when water temperature is 363 K and inlet velocity is 0.1 m/s.

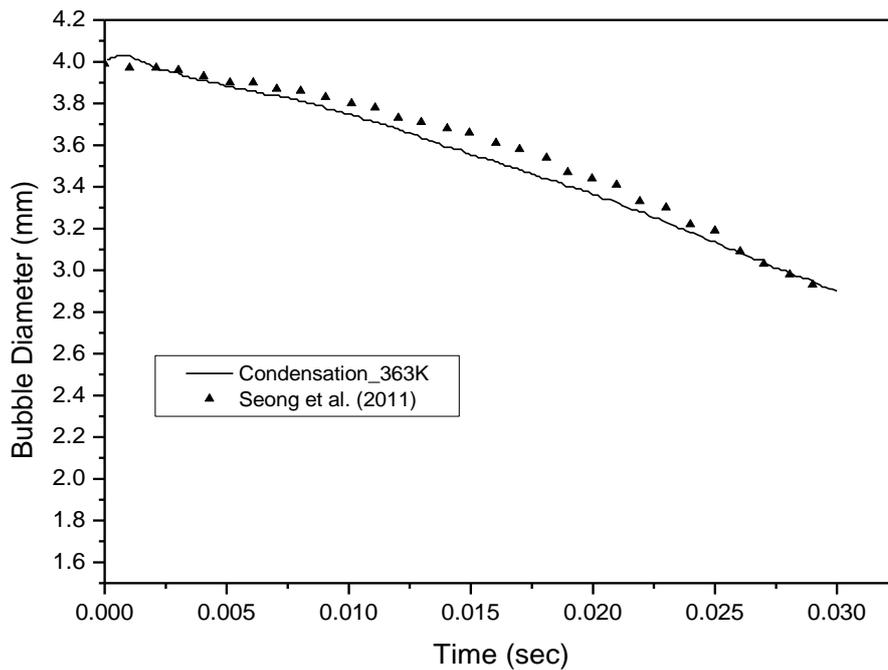


Figure-8 Comparison with results achieved in Fluent code

The results achieved in CFD-ACE+ are in good agreement with those achieved earlier in Fluent code.

8. Conclusion

This report focuses on the simulation of condensation process for a single bubble in subcooled flow boiling regime and a numerical methodology is realized by coupling VOF model with a UDF interface through CFD software CFD-ACE+. The behavior of adiabatic and condensing bubble were studied in 2D simulation and compared to evaluate the capability of developed UDF CFD-ACE+ modeling into the VOF module. For validation of CFD-ACE+ UDF of bubble condensation, an inter code comparison was made and it agreed well with the literature quoted results from FLUENT code. UDF subroutine allows us to customize CFD-ACE+ to fit particular modelling needs. Through this work an emphasis was put on VOF module along with the development of an UDF for bubble condensation in CFD-ACE+ code. This theoretical study is motivated by the future CFD application with 3D simulation. It can be concluded that the VOF model using the CFD-ACE+ modeling for the bubble condensation is a useful computational fluid dynamics tool for analyzing the behavior of the condensing bubble in a wide range of the subcooled boiling flow.

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10. Nomenclature

D_b	=	Bubble diameter
X_{cent}	=	Centre of mass of bubble
ρ	=	Density
μ	=	Dynamic Viscosity
S_h	=	Heat source term

\dot{q}	=	Heat transfer rate
A	=	Interface area
h_{in}	=	Interfacial heat transfer coefficient
Ja	=	Jacob number
h_{fg}	=	Latent heat of vaporization
T_l	=	Liquid temperature
S_α	=	Mass source term
Nu	=	Nusselt number
Pr	=	Prandtl number
U_r	=	Relative velocity of bubble
T_{sat}	=	Saturation Temperature
C_p	=	Specific heat
k	=	Thermal conductivity
\dot{M}	=	Total mass transfer rate
\vec{u}	=	Velocity
α	=	Volume Fraction
$V_{g,j}$	=	Volume of j^{th} gas cell