MODELING FOR FREE SURFACE FLOW WITH PHASE CHANGE

XIAOYONG LUO, MINGJIU NI, ALICE YING, M. ABDOU

Mechanical and Aerospace Engineering Department, UCLA, Los Angeles, CA, 90095, xyluo@ucla.edu

The development of predictive capability for free surface flow with phase change is essential to evaluate liquid wall protection schemes for various fusion chambers in IFE and MFE. This paper presents a numerical methodology for free surface flow with heat and mass transfer to help resolve feasibility issues encountered in the aforementioned fusion engineering fields. The numerical methodology is conducted within the framework of the incompressible flow with the heat and mass transfer model. We present a new second-order projection method, in conjunction with Approximate-Factorization techniques (AF method) for incompressible Navier-Stokes equations. The level set method was used to capture the free surface of the flow and the deformation of the droplets accurately. This numerical investigation identifies the physics characterizing transient heat and mass transfer of the droplet and the free surface flow. The preliminary results show that the numerical methodology is successful in modeling the free surface with heat and mass transfer, though some severe deformation such as breaking and merging occurs. The versatility of the numerical methodology shows that the work can easily handle complex physical conditions in fusion science and engineering.

I. INTRODUCTION

Development of predictive capability for free surface flow with phase change is essential to evaluate liquid wall protection schemes for various fusion chambers. In IFE, the x-ray flux hits the first wall surface first. The energy deposits in depths of a few micrometers and vaporizes the surface. A small fraction of the mass evaporated within the chamber is less energetic and disperses within the chamber volume, raising the pressure significantly. However, the available surface area is expected to be too small to produce sufficiently rapid condensation to restore the required vacuum for Heavy-Ion propagation for the next shot within the allowed 0.167 s for a 6 Hz repetition rate. Cold flibe is sprayed into the annular region between the flibe blanket and the vessel wall to condense the vapors. Using a conservative approach, it is assumed that the spray must absorb all x-ray and debris energy (112 MJ) and restore the required vapor density to $3x10^{13}$ cm^{-3}. Accurate prediction of the spray drop condensation rate is required to insure that condensation occurs rapidly enough to achieve the desired repetition frequency of 6 Hertz. In MFE, the main issue of the liquid wall concept is the compatibility of a free surface liquid with the plasma. Plasma compatibility will likely set a limit on the amount of material allowed to evaporate or sputter from the surface. This evaporation limit will in turn give a surface temperature limit of the flowing liquid layer. Strategies to minimize evaporation from the liquid wall will need to minimize the surface temperature. An integrated droplet-type divertor has been considered in the CLiFF design in order to create higher heat removal capability. One idea is to inject droplets so they strike the liquid surface at an acute angle and merge with the flow to enhance the heat transfer of the liquid walls. However, there has not been much research about the critical issues for this approach.

The numerical simulation of free surface flow with phase change has made only slow progress, although it has become an active topic during the past years. Son and Dhir [1] employed the projection method to do numerical simulation of boiling heat transfer, which incorporates the level set approach for capturing the interface. The first-order fully explicit and full implicit schemes are employed to update the convective and diffusion terms respectively. The temporal accuracy of the schemes in [1] is only first-order. Bai and Schrock [2] use an approximate method for analyzing transient condensation on spray in HYLIFE-II which led to the design selection of 2 mm diameter drops sprayed at a temperature of 843 K and a flow rate of $2.4x10^{3}$ kg/s. However, their model does not fully address the two-phase flow phase change problem since they have many assumptions: the surfaces of the droplets are always at the saturation temperature; the flow distribution inside the droplet is constant; thermal resistance of condensate is neglected; external effect of vapor mass transport is neglected; distortions of the droplet shape are neglected; the change in the droplet size is neglected; internal convection inside the droplet is neglected; gravitational effects are neglected and the droplets are assumed at uniform speed. The proposed work will perform a more sophisticated numerical simulation for this kind of problem to provide more accurate and reliable information.

This paper presents a numerical methodology which is being conducted by using the second-order projection method, in conjunction with Approximate-

Factorization techniques (AF method), for incompressible Navier-Stokes equations. The Crank-Nicholson method was used for the diffusion term to eliminate the numerical viscous stability restriction and third-order ENO scheme used for the convective term to guarantee the accuracy of the method. A four-level V cycle multi-grid algorithm for pressure Poisson equation is used in order to decrease computation time. To capture the free surface of the flow and the deformation of the droplets accurately, we use the level set method by S. Osher and J.A. Sethian [3]. The level set approach has two inherent strengths. One very useful feature is that the representation of the interface as the level set of some function leads to convenient formulas for the interface normal direction and curvature. Another advantage of this approach is that no special procedures are required in order to model topological changes of the front.

The objective of this work is to develop numerical schemes for free surface flow with heat and mass transfer to help resolve feasibility issues encountered in fusion engineering science, specifically in spray droplet condensation efficiency in IFE and on heat removal capability of free surface flow divertor in MFE. The preliminary results show a vaporization modeling case and a rapid condensation case in HYLIFE-II.

II. NUMERICAL MODELING

For incompressible multi-phase flows with phase change, the governing equations can be written as

$$\nabla \cdot \vec{u} = \frac{Ja}{Pe}\left[\frac{\widetilde{K}}{\widetilde{\rho}^2}\left(\nabla T \cdot \nabla \widetilde{\rho}\right)\right] \tag{1}$$

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \left(\vec{u}\,\vec{u}\right) = -\frac{1}{\widetilde{\rho}}\nabla p + \left(\frac{1}{Fr} - \frac{Gr}{\mathrm{Re}^2}T\right)\vec{g} + \frac{1}{\widetilde{\rho}\,\mathrm{Re}}\nabla \cdot \left(\widetilde{\mu}\nabla \vec{u}\right) + \frac{1}{\widetilde{\rho}\,\mathrm{Re}}\nabla \cdot \left(\widetilde{\mu}\nabla \vec{u}\right)^T + \frac{k(\phi)\delta(\phi)\nabla\phi}{\widetilde{\rho}We} \tag{2}$$

$$\frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T = \frac{1}{\widetilde{\rho}\widetilde{C}_p}\frac{1}{Pe}\left[\nabla \cdot \left(\widetilde{K}\nabla T\right)\right] \tag{3}$$

with dimensionless groups of Reynolds, Froude, Weber, Pelect, Jacob, and Grashof numbers as

$$\mathrm{Re} = \frac{\rho_l UL}{\mu_l},\ Fr = \frac{U^2}{gL},\ We = \frac{\rho_l U^2 L}{\sigma},\ Pe = \frac{\rho_l ULC_{pl}}{K_l}$$

$$Ja = \frac{Cpl\left(T_w - T_{sat}\right)}{h_{fg}},\ Gr = \frac{g_0 L^3 \rho_l^2 \beta_l \left(T_w - T_s\right)}{\mu_l^2}.$$

Here $\widetilde{\mu} = \mu/\mu_l$, $\widetilde{\rho} = \rho/\rho_l$, $\widetilde{K} = K/K_l$, and $\widetilde{C}_p = C_p/C_{pl}$ are the dimensionless ratios of the viscosity, density, thermal conductivity and specific heat, ϕ is the level set function, k is the curvature of the interface and δ is the smeared-out Dirac delta function. A continuum surface force (CSF) model is used to reformulate the surface tension as a volume force.

To capture the free surface of the flow and the deformation of the droplets accurately, we use the level set method as follows:

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0 \tag{4}$$

To prevent instability, it is necessary to smooth the values of the density ρ and viscosity μ as

$$\rho_\xi(\phi) = \lambda_\rho + (1-\lambda_\rho)H_\xi(\phi) \tag{5}$$

$$\mu_\xi(\phi) = \lambda_\mu + (1-\lambda_\mu)H_\xi(\phi) \tag{6}$$

where $\lambda_\rho = \rho_g/\rho_l$ and $\lambda_\mu = \mu_g/\mu_l$. H is the smeared out Heaviside function defined by:

$$H(\phi) = \begin{cases} 0 & \phi < -\varepsilon \\ \frac{1}{2} + \frac{\phi}{2\varepsilon} + \frac{1}{2\pi}\sin\left(\frac{\pi\phi}{\varepsilon}\right) & -\varepsilon \le \phi \le \varepsilon \\ 1 & \phi < \varepsilon \end{cases} \tag{7}$$

where ε is a tunable parameter that determines the size of the bandwidth of numerical smearing. A typically good value is $\varepsilon = 1.5\Delta x$, see Figure 1.

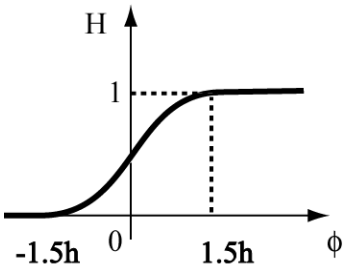


Figure 1. Smooth of the Heaviside function

In this work, we extend the RKCN high-accuracy projection method [4] to the variable-density unsteady incompressible N-S equations, incorporating a level set equation for the interfacial flows. Crank-Nicholson implicit technique is employed to update the diffusion term for stability and the low-storage three-stage Runge-Kutta technique is employed to update the convective term for simplicity and stability. The projection method also has second-order temporal accuracy for variable-density unsteady incompressible flows. The diffusion term can be spatially discretized using standard central difference schemes. The convective term in the momentum equation can be conveniently updated using the third-order ENO scheme.

III. MASS TRANSFER MODELING

The mass transfer during the phase change process is associated with the temperature and density gradient near the interface, as we can see from the governing equation (1). Since the interface usually has a fairly complex shape, the level set representation of the interface is used in this work. Taking the subcell location of the interface into account allows us to discretize the temperature gradient more accurately. Assume the interface lies between the nodes i and i+1 and the temperature at these nodes are T_i and T_{i+1} respectively (see Figure 2). Define a θ function to estimate the subcell interface location:

$$\theta = \frac{|\phi_i|}{|\phi_i + \phi_{i+1}|} \tag{8}$$

The interface splits this cell into two pieces of size $\theta\Delta x$ on the left and size $(1-\theta)\Delta x$ on the right. Denoting the temperature value at this subcell interface location by T_I, which is given by the physical properties and discretizing the temperature gradient near the interface as

$$\left(\frac{\partial T}{\partial x}\right)_{liquid} = \frac{T_{i+1} - T_I}{(1-\theta)\Delta x}, \left(\frac{\partial T}{\partial x}\right)_{Gas} = \frac{T_I - T_i}{\theta\Delta x} \tag{9}$$

To get the second derivative of the temperature across the interface, we know

$$(KT_x)_{i+1/2} = K^-\left(\frac{T_I - T_i}{\theta\Delta x}\right) \tag{10}$$

$$(KT_x)_{i-1/2} = K^-\left(\frac{T_i - T_{i-1}}{\theta\Delta x}\right) \tag{11}$$

So

$$\frac{\partial}{\partial x}(KT_x)_i = \frac{(KT_x)_{i+1/2} - (KT_x)_{i-1/2}}{\Delta x} \tag{12}$$

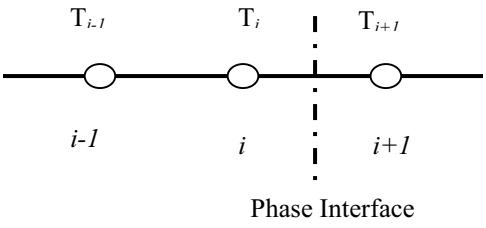


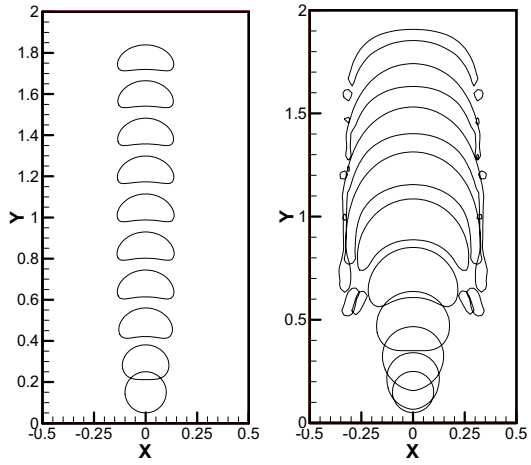
Figure 2. Phase interface location

IV. NUMERICAL RESULTS

To test the validity of the numerical methodology, we perform the numerical simulation on various validation cases to benchmark it and furthermore to predict the heat and mass transfer process in fusion science and engineering precisely. In this paper we will present a vaporization modeling case and a rapid condensation modeling case in HYLIFE-II environment.

IV. A. Vaporization case

The two-dimensional single bubble computational domain is 1×2 and the meshes are 57×103. The initial bubble radius is 0.1. The Reynolds number is 100 and the Weber number is 5. The density ratio is $\rho_l/\rho_g = 1000/1$ and the viscosity ratio is $\mu_l/\mu_g = 100/1$. To initiate the computations, the initial fluid temperature profile is taken to be linear in the natural convection thermal boundary layer and fluid velocity is set equal to zero. The initial thermal boundary layer thickness is assumed to be 1 in this case. Figure 3 shows the bubble growth pattern with time when $\Delta T = 6.2K$ compare with no heat and mass transfer. With the heat and mass transfer, the bubble grows fast when under thermal boundary layer. After that, the bubble grows slow and begins to break into smaller bubbles.



(a) No heat and mass transfer (b) with heat and mass transfer

Figure 3. Comparison of single bubble growth pattern

Figure 4 shows the bubble mass change with computational steps. The dash line is the result when there in no heat and mass transfer while the solid line is the results when there is heat and mass transfer. The bubble mass increases almost six times compared with initial time when heat and mass transfer occurs. When the bubble moves above the thermal boundary layer, the mass increase speed decreases because of temperature difference is decreased.

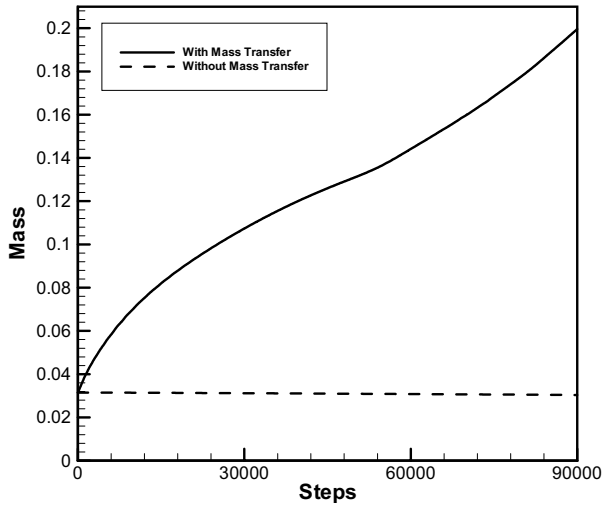


Figure 4. Bubble mass changes with computational steps

IV. B. Rapid condensation case

Peterson et.al [5] did the first numerical study of condensation on liquid droplets under the HYLIFE-II environment. Bai and Schrock [2] perform a detailed analysis of the temperature profile in the droplet. In this paper, we perform the full numerical simulation on the droplet and assume the surfaces of droplets are always at the saturation temperature corresponding to the instantaneous vapor pressure. We assume the surface temperature difference of the droplet to be exponentially decaying with time

$$T_{sat}(t) = T_0 e^{-\tau/t_0} \tag{13}$$

where T_0 is the step temperature rise at t=0.

In this paper, the physical properties of the liquid Flibe ($(LiF)_2(BeF_2)$) is from [6]. Unfortunately there are no physical properties data available for the gas Flibe. Here we use Lennard-Jones potential in the Chapman-Enskog kinetic theory of gases to get dynamic viscosity and thermal conductivity:

$$\mu = 2.67\times10^{-6}\frac{\sqrt{MT}}{\sigma^2\Omega_\mu} \tag{14}$$

$$K_{translational} = 8.32\times10^{-2}\frac{\sqrt{T/M}}{\sigma^2\Omega_k} \tag{15}$$

Where σ is the collision diameter, Ω is the collision integral.

The equation is valid for monatomic gases; for polyatomic gases we add the modified Eucken correction to account for the contribution of the internal degrees of freedom:

$$K = K_{translational} + 1.32\left(c_p - \frac{5}{2}\frac{R}{M}\right)\mu \tag{16}$$

The specific heat c_p can be obtained from a simple formula,

$$c_p = (5+N_r)(\frac{1}{2}\frac{R}{M}) \tag{17}$$

where N_r is the number of rotational degrees of freedom. Finally we get the ratio of physical properties of gas and liquid Flibe for the numerical simulation. $\rho_g/\rho_l = 1.99\times10^{-4}$, $\mu_g/\mu_l = 2.9\times10^{-3}$, $C_{pg}/C_{pl} = 0.422$, $k_g/k_l = 0.037$.

Figure 5 shows the average temperature rise of a drop diameter of 5mm and 10mm with time. τ is set to be equal to 40ms and 80ms separately. We turn off the

convection part to compare our results with Bai's. The points are the results from Bai's paper and lines are our numerical results, which match very well. We can see the surface of the drop is rapidly heated initially; however with the vapor temperature exponentially decaying, the temperature gradient at the surface is reduced to zero. Therefore the heat flux is reversed.

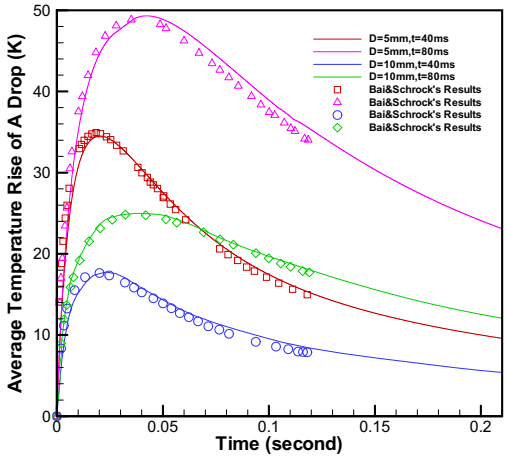


Figure 5. Average drop temperature with time

At the second step, we turn on the convection part since it is known to enhance the heat transfer in this case. Figure 6 shows the results of average drop temperature with/out convection for D=5mm t=40ms case. We only compare the first 0.025 second result since there is a condensation process during this period. The average temperature increase 10% with the convection part.

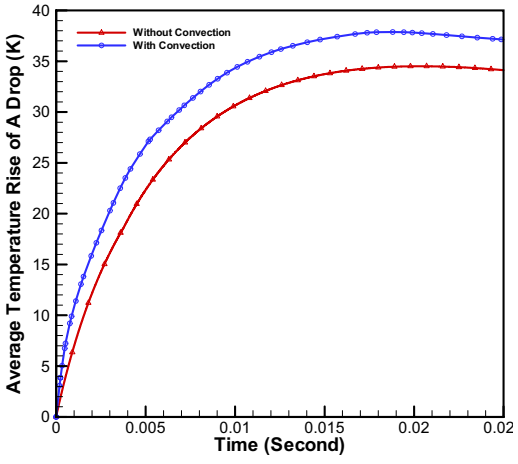


Figure 6. Comparison of average drop temperature with/out convection

V. CONCLUSION

This work has presented the modeling development for the free surface flow with heat and mass transfer. A new second-order projection method has been used to solve the two-phase incompressible flow Navier-Stokes equations. Crank-Nicholson method for the diffusion term was used to eliminate the numerical viscous stability restriction and high order ENO scheme for the convective term to guarantee the accuracy of the method. The level set method is incorporated in this work in order to compute and analyze the motion of an interface, including the free surface of the flow and the bubble or liquid droplet topological changes such as breaking and merging. The preliminary results show the numerical methodology is successful in modeling the free surface with heat and mass transfer even if some severe deformation such as breaking and merging happens. The versatility of the numerical methodology shows the work can easily handle complex physical conditions in fusion science and engineering.

ACKNOWLEDGMENTS

This work is supported by the U.S. Department of Energy under Grant No. DE-FG03-86ER52123.

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