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Application of the level set method for multi-phase flow computation in fusion engineering

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Abstract

Numerical simulation of multi-phase flow is essential to evaluate the feasibility of a liquid protection scheme for the power plant chamber. The level set method is one of the best methods for computing and analyzing the motion of interface among the multi-phase flow. This paper presents a general formula for the second-order projection method combined with the level set method to simulate unsteady incompressible multi-phase flow with/out phase change flow encountered in fusion science and engineering. The third-order ENO scheme and second-order semi-implicit Crank–Nicholson scheme is used to update the convective and diffusion term. The numerical results show this method can handle the complex deformation of the interface and the effect of liquid–vapor phase change will be included in the future work.

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1. Introduction

There are many liquid wall conceptions that have been designed for the magnetic fusion energy plant, such as the convective liquid flow first-wall concept (CliFF) [2]. The idea behind the CliFF is to eliminate the presence of a solid first wall (FW) facing the plasma through which the surface heat load must conduct. This goal is accomplished by means of a fast moving thin liquid layer flowing on the

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FW surface. The layer adheres to the curved wall by means of its centrifugal acceleration, U^2/R , where U is the velocity and R is the radius of the curvature of the first structural wall surface. This thin layer is easier to control than a thick liquid FW/Blanket, but still provides a renewable liquid surface immune to radiation damage and sputtering concerns. It also largely eliminates thermal stresses and its associated problems in the first structural wall. The liquid film can be utilized at the bottom of the reactor as an integrated liquid surface divertor, and then removed from the vacuum chamber by gravity drainage, an EM pump, or some more sophisticated heat recovery system.

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Fig. 1. Schematic of CliFF implementation in ARIES-RS scale reactor.

The general CliFF design [2], as seen in Fig. 1, is conceptually simple in its implementation. A thin fast liquid layer is injected near the top of the plasma chamber. The layer flows down the reactor walls without excessive slowing down or thinning out, and is removed in some fashion from the bottom of the chamber. Layer thickness h on the order of 0.5-2 cm, and velocities U on the order of 10 m/s, are considered for three different working liquids; Li, Sn-Li and the molten salt Flibe. The main issue of the liquid wall concept in this design 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 to 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 critical issues relative to this approach since very complicated interface phenomena involved. How to capture the dynamics of the interface by numerical simulation plays a key role in this research project.

There are two basic approaches that can be used to approximate flows with a material interface: "capturing" and "tracking". In interface capturing, the interface is treated as a region of steep gradient in some quantity (e.g. density) that satisfies an advection equation. The primary advantages of this approach are that it is easy to implement and no additional algorithmic details are required to model topological changes of the interface. However, the front diffuses over several computational zones, resulting in a corresponding loss of accuracy. In an interface tracking method, the interface is treated explicitly as a sharp discontinuity moving through the grid. Tracking can offer better accuracy than capturing, but at the cost of greater algorithmic complexity. There are basically three possible representations of an interface with an interface tracking method: level set methods; volume-of-fluid (VOF) methods and "front tracking"; and boundary integral methods. What follows is a summary of methods that is pertinent to the current work.

The key idea of level set method, as devised in 1987 by Osher and Sethian [1] for dynamic implicit surfaces, is the Hamilton-Jacobi approach to numerical solutions of a time dependent equation for a moving implicit surface. The earliest real success in the coupling of the level set method to problems involving external physics (Sussman et al. [3]) comes in computing two-phase incompressible flow. In this paper, the surface tension term is considered to be a force concentrated on the interface by using the continuum surface force (CSF) model. In 1999, Sussman and Fatemi [4] formulated a constraint designed to prevent the straying of the zero level set from the initial position even after many iterations which improves the accuracy of the redistance iteration. This in turn helps when applied to the basic advection of a level set function and when applied to interfacial incompressible flow.

The objective of this work is to develop a general formula for the second-order projection method combined with the level set method to simulate unsteady incompressible multi-phase flow without phase change flows. The numerical simulation results will help resolve feasibility issues encountered in fusion engineering science, specifically in heat removal capability of free surface flow divertor in magnetic fusion energy (MFE).

2. Numerical modelling

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

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

$$\frac{\partial u}{\partial t} + \nabla \cdot (\vec{u}\vec{u})$$

$$= -\frac{1}{\tilde{\rho}}\nabla p + \left(\frac{1}{Fr} - \frac{Gr}{Re^2}T\right)\vec{g} + \frac{1}{\tilde{\rho}Re}\nabla \cdot (\tilde{\mu}\nabla\vec{u})$$

$$+ \frac{1}{\tilde{\rho}Re}\nabla \cdot (\tilde{\mu}\nabla\vec{u})^{\mathrm{T}} + \frac{k(\phi)\delta(\phi)\nabla\phi}{\tilde{\rho}We}$$
(2)

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

where

$$[\nabla T]_{\Gamma} = (\nabla T)_{\text{liquid}} - (\nabla T)_{\text{gas}} \tag{4}$$

with dimensionless groups of Reynolds, Froude, Weber, Jacob, Pelect and Grashof numbers. $Re = \frac{\rho_l UL}{\mu_l}$, $Fr = \frac{U^2}{gL}$, $We = \frac{\rho_l U^2 L}{\sigma}$, $Ja = \frac{Cpl(T_w - T_{sat})}{h_{fg}}$, $Pe = \frac{\rho_l ULC_{pl}}{K_l}$, $Gr = \frac{g_0 L^3 \rho_l^2 \beta_l (T_w - T_s)}{\mu_l^2}$, where *U* and *L* are characteristic velocity and length, respectively; σ the surface tension coefficient; $\tilde{\mu} = \mu/\mu_l$, $\tilde{\rho} = \rho/\rho_l$, $\tilde{K} = K/K_l$, and $\tilde{C}_p = C_p/C_{pl}$ the dimensionless ratios of the viscosity, density, thermal conductivity and specific heat, ϕ the level set function, *k* the front 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.

The level set method [1] is employed to capture the interface implicitly by introducing a smooth level set function ϕ , with the zero level set as the interface and positive value outside interface and negative value inside the interface. The evolution of the implicit function $\phi(\leftarrow x, t)$ is governed by the simple convection equation, sometimes referred to as the level set equation:

$$\frac{\partial \phi}{\partial t} + \vec{u} \cdot \nabla \phi = 0 \tag{5}$$

This is an Eulerian formulation of the interface evolution since the interface is captured by the implicit function $\phi(\leftarrow x, t)$ as opposed to being tracked by interface elements as in a Lagrangian formulation. While Eq. (5) will move the level set $\phi = 0$ at the correct velocity, ϕ will generally drift away from its initialized value as signed distance, i.e. ϕ will no longer be a distance function. Sussman and Fatemi [4] consider the following function $\phi_0(\vec{x})$ whose zero level set is the air–liquid interface; $\phi_0(\vec{x})$ need not be a distance function, however. They construct a function, $\phi(\vec{x})$, with the properties that its zero level set is the same as $\phi_0(\vec{x})$ and that ϕ is the signed normal distance to the interface. This is achieved by solving the following problem to a steady state

$$\phi_t = L(\phi_0, \phi) = S_{\varepsilon}(\phi_0)(1 - |\nabla \phi|) \tag{6}$$

$$|\nabla\phi| = \sqrt{\phi_x^2 + \phi_y^2 + \phi_z^2} \tag{7}$$

where $S(\phi_0)$ is a sign distance function taken as 1 in Ω^+ , -1 in Ω^- , and 0 on the interface, where ϕ stays identically equal to zero. For numerical purposes it is useful to smooth the signed function as

$$S_{\varepsilon}(\phi_0) = \frac{\phi_0}{\sqrt{\phi_0^2 + \varepsilon^2}} \tag{8}$$

Eq. (6) has the property that ϕ remains unchanged at the interface; therefore, the zero level set of ϕ_0 and ϕ are the same. Away from the interface, ϕ will converge to $|\nabla \phi| = 1$, which means it will converge to the actual distance. By using this equation, there is no need to initialize any points near the interface for use as boundary conditions. The points near the interface in Ω^+ use the points in Ω^- as boundary conditions, while the points in Ω^- conversely look at those in Ω^+ . This circular loop of dependencies eventually balances out, and a steadystate singed distance function is obtained. This method works rather well as long as ϕ is relatively smooth and the initial data are somewhat balanced across the interface.

Ideally, the interface remains stationary during the reinitialization procedure, but numerical errors will tend to move it to some degree. Thus, the Eq. (6) cannot conserve the volume of the domain bounded by the curve defined implicitly by the level set function $\phi_0(\vec{x})$. In [4], Sussman and Fatemi suggested an improvement to the standard reinitialization procedure to preserve the mass in each cell by a local constraint. This local constraint is implemented by adding a correction term to the right side of Eq. (6).

$$\phi_t = L(\phi_0, \phi) + \lambda f(\phi) \tag{9}$$

where λ is a function of *t* only, determined by

$$\lambda = \frac{-\int_{\Omega} H'(\phi) L(\phi_0, \phi)}{\int_{\Omega} H'(\phi) f(\phi)}$$
(10)

where

$$f(\phi) = H'(\phi) |\nabla \phi| \tag{11}$$

This ensures that we correct only at the interface, without disturbing the distance function property away from the interface. In this work, λ is calculated for each grid cell. We use a 9-point quadrate formula to evaluate the integrals in two spatial dimensions and 27-point quadrate formula in three spatial dimensions.

$$\int_{\Omega_{ij}} g \approx \frac{h^2}{24} \left(16g_{ij} + \sum_{m,n=-1;(m,n)\neq(0,0)}^{1} g_{i+m,j+n} \right)$$
(12)

It is shown that this specific discretization exactly cancels out a first-order error term introduced in the previous formulation.

In this work, we extend the RKCN highaccuracy projection method [5] to the variable-density unsteady incompressible N–S equations, incorporating a level set equation for the interfacial flows [6]. 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 thirdorder ENO scheme.

3. Numerical results

To test the validity of the numerical methodology, we perform the numerical simulation on various validation cases. In this paper, we will present single droplet spray and multiple droplets spray modeling cases. The physical properties are based on the data of Flibe [6]. The density ratio is $\rho_g/\rho_l = 1.99 \times 10^{-4}$, $\mu_g/\mu_l = 2.9 \times 10^{-3}$. The three-dimensional computational domain is $25 \text{ mm} \times 25 \text{ mm} \times 25 \text{ mm}$ and the meshes are $57 \times 57 \times 57$. The Reynolds number is 100 and the Weber number is 5. The initial velocity of the droplet is zero in all three cases.

3.1. Single droplet spray modeling

In the single spray droplet case, the initial bubble radius is 2.5 mm and located at z = 20 mm while below z = 6.25 mm are all filled with liquid.

Fig. 2 shows the dynamics of droplet interaction with the free surface. Because of the small Weber number, surface tension is pretty high. The surface tension force causes oscillation of the free surface flow as high as 5.13 mm. That is, the surface tension



Fig. 2. Large Flibe droplet sprayed onto a free surface through the gas phase.

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Fig. 3. Three large Flibe droplets sprayed onto a free surface through the gas phase.



Fig. 4. Two layer three large Flibe droplets sprayed onto a free surface through the gas phase.

energy is converted to kinetic energy of fluid motion. This motion will be very effective in keeping the surface temperature down which, in turn, will lower the evaporation rate. More results about the heat transfer associated with the mixing flow will be given in the future.

3.2. Multiple droplets spray modeling

In the multiple droplets case, the initial three bubbles' radii are 2.5 mm each and form an equilateral triangle. These three droplets are located at z = 20 mm while those below z = 6.25 mm are all filled with liquid.

Fig. 3 shows the dynamics of three droplets interacting with the free surface. The surface tension force causes the oscillation of the free surface flow to be as high as 6.03 mm. This is a little higher than the single droplet case because of the interaction between these droplets. This oscillation height must be controlled since oscillation which is too high or a splash will pollute the chamber. The velocity of the droplets is about 0.5 m/s when the droplets hit the free surface.

3.3. Two-layer multiple droplets spray modeling

The initial six bubbles' radii are 2.5 mm each and form an equilateral triangle of two layers each. The upper layer is located at z = 20 mm and the lower layer is located at z = 12.5 mm. Those below z = 6.25 mm are all filled with liquid.

Fig. 4 shows the dynamics of what happens when the lower layer three droplets hit the free surface first and the upper layer three droplets hit thereafter. The oscillation height is about 6.47 mm. This is higher than in the previous case because the free surface is subsequently hit by large liquid droplets. More discussion about the effects of droplet radius, the initial velocity of the droplet, the

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height of the initial droplet, no droplet ejection condition or "no splash" condition will be given in the future.

4. Conclusion

A level set method combined with the second-order RKCN projection method for the multi-phase incompressible flow was developed and applied to a free surface flow divertor concept. Crank-Nicholson method for the diffusion term was used to eliminate the numerical viscous stability restriction. The high order ENO scheme was used for the convective term to guarantee the accuracy of the method. The results show the numerical methodology is successful in modeling the hydrodynamics of the multi-phase flow even if severe surface deformation occurs. More results about the heat transfer associated with the mixing flow will be given in the future. The versatility of the numerical methodology shows the work can handle complex physical phenomena encountered in fusion engineering sciences.

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