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A coupled vaporization model based on temperature/species gradients for detailed numerical simulations using conservative level set method

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ABSTRACT

This paper proposes a vaporization model for detailed numerical simulations of a reactive interface. The proposed model represents a preliminary attempt to combine vaporization models based on heat flux and species mass flux to take each model's advantages concerning numerical accuracy, robustness and applicability. We utilize a conservative level set method to reduce unphysical mass loss in capturing the deformable interface, and the ghost fluid method to accurately impose various jump conditions across the interface. Four validations are conducted to demonstrate both the strengths and limitations of the two original models. Since the vapor mass fraction is relevant in realistic applications, we add the species solver to the heat flux based model and assess the coupling strategy in different situations. The feasibility of switching between the two frameworks in the coupled vaporization model is also demonstrated. Finally, the coupled model is applied to simulations of deformable/moving droplet under high-ambient-temperature conditions. The results of the simulations are consistent with analytical and experimental data. Although additional work is required, the coupled vaporization model exhibits potential as a means for modeling spray combustion.

1. Introduction

The vaporization process is among the most common heat and mass transfer phenomena and plays a critical role in many nature and technical applications. Examples of this process include liquid evaporation from oceans and clouds, boiling in boilers and burning in combustion chambers. Since the energy industry seeks to improve system efficiency and serving life, it is always of great interest to explore the intrinsic mechanisms of vaporization. However, the small spatial and temporal scales involved in vaporization cause technical challenges for experimental tools. Alternatively, high-resolution numerical methods have exhibited potential as a promising tool. Their use may lead to novel insights into the fundamental physics.

Over the past two decades, researchers have devoted considerable effort to modeling gas-liquid flows [1–4], in which the interface moves, deforms and breaks up over time. The challenges in such simulations lie in the specific treatments of complex interface evolution, various jump conditions across the interface and the singularity of surface tension. Simulations of vaporizing gas-liquid flows are even more challenging because a local flow, i.e., Stefan flow, emerges near the interface. The Stefan flow results in new jump conditions across the interface and increases the complexity of those already present. A framework of detailed numerical simulation (DNS) in conjunction with a sharp interface method is effective to address these challenges. Numerous interface methods have been proposed in the literature, such as the front tracking (FT) method [5], the arbitrary Lagrangian-Euler method [6], the level set (LS) method [7] and the volume of fluid (VOF) method [8]. The LS method is widely used because of its simplicity and effectiveness. The LS method is probably the easiest to implement for parallelization. According to Tanguy et al. [9], the LS method not only avoids the introduction of a fictitious interface thickness but also improves the resolution of the jump condition by providing accurate discretization of discontinuous terms across the interface. The discontinuities across the interface can be addressed using the ghost fluid method (GFM).

It has been two decades since the pioneering work of Son and Dhir [10], when an interface-resolved DNS method was used to simulate gas-liquid flows with phase change. During this period, many researchers [11–14] have continued to explore vaporization processes, and have reported numerous meaningful conclusions. The literature confirms that interface-resolved DNS methods are promising to investigate vaporization problems. However, further research is still needed before these methods can be eventually

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applied to complex applications. For example, a general and effective method for determining the vaporizing rate is required. For convenience, we refer to methods for calculating vaporization rate as "vaporization models" in this paper. From the perspective of data source, vaporization models can be classified into two categories: the Heat Flux based Model (HFM) and the Species Mass Flux based Model (SMFM).

The HFM of vaporization assumes that the interface stays at the saturation temperature and that the vaporization rate is totally driven by the net conductive heat flux density. When more heat flows into the interface than flows out, the excess heat is absorbed by the liquid near the interface, leading to liquid vaporization. When more heat flows out than flows in, condensation occurs, which is beyond the scope of this paper. In this framework, Son and Dhir [10] modeled a film boiling process on a horizontal surface using the LS method and explored the transition mechanism in bubble release patterns. Luo et al. [15] simulated bubble growth during nucleate boiling using the LS method. Gibou et al. [14] utilized the GFM in combination with the LS method (LS/GFM) for imposing jump conditions across the interface, and they applied the algorithm to film boiling. Similar work was reported in [9,16]. To ease the mass non-conservation issue of traditional LS methods, variants have also been used in this field. In [17,18], a coupled level set and volume of fluid method was utilized to investigate bubble formation and growth in boiling processes. Lee et al. [19] proposed an improved LS-based approach for multiphase flows with phase change. The authors focused on reducing the potential numerical errors from unphysical pressure oscillations, spurious velocity fields and mass flux errors across the interface. Sato and Niceno [20] developed a conservative sharp interface method that is similar to the LS method. The method was used to model a growing vapor bubble in superheated liquid. Additionally, Welch and Wilson [11] used a VOF method to simulate horizontal film boiling. Sun et al. [21] used a VOF method to simulate evaporation and condensation problems. Juric and Tryggvason [22] presented an FT method for film boiling flows. They proposed a general procedure for handling the saturation temperature difference due to the pressure jump across the interface. Esmaeeli and Tryggvason [12] simplified the procedure by defining the saturation temperature at the system pressure as Son and Dhir [10] did.

In contrast to the HFM, the SMFM of vaporization does not involve any restrictive assumptions. Therefore, the SMFM may be applied to more general situations because the species gradient, which is the driving force for vaporization, can interact with the temperature field. In this framework, Tanguy et al. [9] presented a LS/GFM method for vaporizing two-phase flows. Specific care was devoted to the extension of discontinuous variables across the interface to reduce parasitic currents and numerical diffusion. Son [23] simulated microdroplet evaporation on a heated surface using the LS method. He noticed that the sequential calculation procedure of the SMFM was unstable in high evaporation mass flux situations when the denominator in the model is close to zero. He used a Newton–Raphson iterative algorithm in an attempt to restrict the interface temperature and therefore obtain a sufficiently large denominator. However, this modification was not physically correct because the modified interface temperature could not approach the boiling temperature. Duret et al. [24] utilized the LS method to study evaporation and mixing processes in turbulent two-phase flows. We classify their work within the SMFM framework, although they did not explicitly calculate the evaporation rate. Additionally, Schlottke and Weigand [25] presented a VOF method for deformable droplet evaporation. The researchers emphasized correct calculation of velocities near the interface. Strotos et al. [26] employed a VOF method with a local grid refinement technique to investigate the evaporation process of a two-component droplet. A VOF method with a two-scalar approach for heat transfer was also applied by Ma and Bothe [27] to investigate thermocapillary two-phase flows with evaporation.

The HFM and SMFM both exhibit strengths and shortcomings. For example, the HFM has been used for a long time because of its simplicity. However, the applications of the HFM are limited because the interface temperature in this model is constant. Consequently, the model cannot accurately describe the evolution of interface temperature until a steady state has been reached. In the literature, this model is mainly applied to boiling processes. In contrast, the SMFM is applicable to more general problems. For example, the SMFM can deal with water evaporation in air even if the initial temperatures of the two phases are the same and no additional heat source exists. However, the SMFM is relatively fragile and may perform unsatisfactorily in high evaporation mass flux situations. Recently, Rueda Villegas et al. [28,29] linked these two kind of models by solving the mass fraction equation with a prescribed Robin boundary condition on the interface and the energy equation with a non-homogeneous Dirichlet boundary condition. The obtained solver can handle both evaporation and boiling depending on the external condition without requiring any sensors. However, the literature on this topic is scarce. Some researchers [30–33] have used both models in their work. However, these studies focused on topics other than vaporization models, such as developing sharp interface methods and modeling specific problems. Thus, the researchers just used the models separately according to the target applications. The present paper intends to combine the two vaporization models into a coupled model that retains the advantages of the originals and is suitable for more general situations.

The LS/GFM framework is adopted in this work due to its simplicity and effectiveness. However, the original LS methods suffer unphysical mass non-conservation issue in under-resolved regions, which influences the vaporization. This issue for phase change simulations is not as critical as for primary atomization simulations because phase change simulations require sufficiently refined grids to capture the heat and mass transfer boundary layers. However, sufficiently refined grids can only be affordable for small-scale simulations. In large-scale cases, such as spray combustion, the length scale can vary by several orders of magnitude due to liquid breakup and evaporation. Hence the grid resolution is usually inadequate for small structures, and a conservative level set method is preferable in these cases.

The rest of this paper is organized as follows. Section 2 introduces the methodology, including the governing equations and jump conditions. In Section 3, the two original vaporization models and the coupled model are presented. The numerical implements are subsequently discussed in Section 4. Numerical validations and applications are performed in Section 5 to further illustrate the feasibility and limitation of the original models as well as to assess the new model. Finally, conclusions are drawn in Section 6.

2. Mathematical formulation

2.1. Incompressible Navier–Stokes equations

The incompressible Navier–Stokes equations are introduced to describe the conservations of mass and momentum

$$\nabla \cdot \vec{u} = 0, \tag{1}$$

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{\nabla p}{\rho} + \frac{1}{\rho}\nabla \cdot (\mu[\nabla \vec{u} + \nabla \vec{u}^T]) + \vec{g}, \tag{2}$$

where $\vec{u}$ is the velocity vector, p is the pressure, ρ is the density, μ is the dynamic viscosity and $\vec{g}$ is the gravity acceleration.