



DIRECT NUMERICAL SIMULATION OF EVAPORATING SESSILE DROPLETS USING THE ALGEBRAIC VOF APPROACH

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ABSTRACT

This study presents the direct numerical simulation of an evaporating sessile droplet using a sharp-interface algebraic VOF (volume-of-fluid) approach in the finite-volume framework. An interface identification scheme is introduced to determine a sharp layer of interface cells for phase change, and the rate of vaporization is directly computed from the local gradient of vapor mass fractions at the interface, without any tuning parameter in the evaporation model. A solver based on this sharp-interface algebraic VOF approach has been developed in the open-source CFD codes library – OpenFOAM (Open-source Field Operation and Manipulation). The evaporation of a sessile water droplet at the constant contact angle mode was investigated to ensure that the codes have been correctly implemented. The numerical predictions with respect to the squared diameter of the droplet for different values of relative humidity agree well with the experimental data, indicating accurate computation of the evaporation rate. The liquid-vapor interface is found to maintain sharp without obvious smearing, attesting the excellent performance of the interface sharpening scheme. The temperature field in the gas and liquid phase is demonstrated and the well-known local cooling effect caused by evaporation is successfully simulated. The simulation results demonstrate the capability of the present solver in revealing the complex characteristics associated with droplet evaporation, including fluid mechanics and coupled heat and mass transfer.

1. INTRODUCTION

Numerical simulation of evaporating sessile droplets is a challenging task in the computational fluid dynamics (CFD) framework since it involves momentum transport, heat and mass transfer, and moving interface all together. The Hertz-Knudsen-Schrage (HKS) equation has been used to estimate the evaporative flux in simulation of nucleate boiling and evaporating droplets [1-2]. Nikolopoulos et al. [1] numerically investigated evaporation of n-heptane and water liquid droplets using the classical HKS evaporation model. Chen et al. [2] developed a similar model based on the HKS equation to determine the evaporative flux and investigated the evaporation cooling mechanism of water droplets impacted onto heated surfaces. However, one adverse factor of the HKS-based evaporation model is the uncertainty in its thermal accommodation coefficient, and determination of this coefficient requires a troublesome trial-and-error procedure to align with the experimental data.

A more general method to evaluate evaporation rates was proposed by Schlottke and Weigand [3]. This method employs direct numerical simulation (DNS) to determine evaporation rates without any empirical input. Central to this method is geometric reconstruction of liquid-vapor interfaces, i.e., geometric VOF (volume-of-fluid) method, as it is required in DNS calculations of evaporative source terms. However, the geometric VOF method is disadvantageous due to expensive computational costs and unease of use in arbitrary unstructured meshes. Plus, the algorithm to calculate spatial gradients is complicated due to discontinuous physical variables at the interface. Alternatively, the algebraic VOF method tracks the moving interface by discretizing the transport equation of volume fractions using a differencing scheme. This method presents the advantages of simplicity, high robustness, fast convergence and applicability to unstructured meshes. However, the algebraic VOF method does not involve explicit reconstruction of liquid-vapor interfaces but instead gives a “region” of interface, a disadvantage requiring special treatment if one was to incorporate the algebraic VOF with the DNS approach.

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In the present study, we employ the algebraic VOF method for direct numerical simulation of evaporating sessile droplets in an inert gas. The liquid-vapor interface necessary for the DNS modelling of evaporation is explicitly identified from interface cells, and phase change is restricted to take place only in the interface cells. Finally, the developed solver is validated by a case study of an evaporating sessile droplet on a hydrophobic substrate.

2. MATHEMATICAL FORMULATIONS

A volume fraction α_i is the partial volume of phase i in a control volume and here i takes 1, 2, 3 for liquid, vapor, and the inert gas, respectively. Assuming incompressible and Newtonian flows, the transport equations for the volume fraction of liquid and vapor are given by

$$\frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 \vec{U}) = -\frac{\dot{m}}{\rho_1} \quad (1a)$$

$$\frac{\partial \alpha_2}{\partial t} + \nabla \cdot (\alpha_2 \vec{U}) = \nabla \cdot (D \nabla \alpha_2) + \frac{\dot{m}}{\rho_2} \quad (1b)$$

where \vec{U} , ρ_i , \dot{m} and D denote velocity, density of phase i , evaporation rate and diffusivity, respectively. The volume fraction of the inert gas, α_3 , is given by $1 - \alpha_1 - \alpha_2$.

The conservation equations for momentum and energy are respectively described by

$$\frac{\partial(\rho \vec{U})}{\partial t} + \nabla \cdot (\rho \vec{U} \vec{U}) = -\nabla p + \nabla \cdot [\mu(\nabla \vec{U} + \nabla^T \vec{U})] + \rho \vec{g} + \vec{f}_\sigma \quad (2)$$

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot (\rho \vec{U} c_p T) = \nabla \cdot (k \nabla T) + \Delta h_{ev} \dot{m} \quad (3)$$

where p , μ , \vec{g} and \vec{f}_σ in Eq. (2) represent pressure, dynamic viscosity, gravitational acceleration and surface tension force, respectively; T , c_p , k and Δh_{ev} in Eq. (3) denote temperature, specific heat capacity, thermal conductivity and latent heat of vaporization, respectively.

3. NUMERICAL METHODOLOGY

3.1 Reconstruction of Sharp Interface

In the algebraic VOF method, the liquid-vapor interface is not represented as an explicit boundary separating the two phases but instead several layers of computational cells where the liquid volume fraction ranges from 0 to 1. In this work, a specific interface identification scheme reported in [4] is used to determine a sharp layer of interface cells explicitly. A detailed description of the interface identification procedure can be referred to [4].

3.2 Calculation of Evaporative Flux

The evaporative flux in the interface cells is calculated directly from the local gradient of the vapor mass fraction X_V ,

$$\dot{m}'' = \frac{\rho_{gp} D}{1 - X_V} \langle \nabla X_V \cdot \vec{n} \rangle \quad (4)$$

where ρ_{gp} is the density of gas mixture and $\langle \cdot \rangle$ denotes the inner product.

A special scheme is employed to associate each interface cell with its closest neighbour cell in the gaseous phase along the normal direction of the interface, which ensures the single-sided calculation for spatial gradients. Indicating with the subscript *int* an interface cell and with *nei* its closest neighbouring cell, we can express the mass flux of vapor as,

$$\dot{m}'' = \frac{\rho_{gp} D}{1 - X_{V,int}} \frac{X_{V,int} - X_{V,nei}}{|\vec{d}|} \frac{\langle \vec{d} \cdot \vec{n}_V \rangle}{|\vec{d}|} \quad (5)$$

where \vec{n}_V is a unit vector normal to the interface, pointing from liquid to vapor, and \vec{d} is the distance vector connecting the interface cell and its corresponding neighboring cell. The details can be referred to [4].

3.3 Calculation of Surface Tension Force

The continuous surface force (CSF) model has been employed in the present study to calculate the surface tension force and the phase-indicator field is smoothed to minimize the parasitic currents caused by discretization errors. The smoothing is only performed to calculate the surface tension force and thus has no influence on the actual liquid distribution.

Given the interface density expressed by $|\nabla\alpha_1|$, the surface tension force is computed by

$$\vec{f}_\sigma = \sigma \kappa_s \nabla\alpha_1 \quad (6)$$

The sharp-interface algebraic VOF approach was implemented in the finite-volume based CFD code package – OpenFOAM and a solver was developed. The MULES (Multidimensional Universal Limiter with Explicit Solution) method was used to solve the volume fraction equations of liquid and vapor, and the compressive differencing scheme was employed to maintain high resolution of the interface. The pressure velocity coupling was handled by the PIMPLE algorithm, which is a combination of SIMPLE (Semi-Implicit Method for Pressure Linked Equations) and PISO (Pressure-Implicit with Splitting of Operators) loop.

4. VALIDATION CASE

The sharp-interface algebraic VOF solver was validated against the experimental data for evaporation of sessile droplets sitting on a hydrophobic substrate in the constant contact angle (CCA) mode [5]. The evaporation occurs in ambient conditions with a constant temperature (298 K) and pressure (101325 Pa). The sessile water droplets with an initial volume of 3 μL are exposed to the ambient air at different values of relative humidity (RH = 10%, 30% and 50%) as shown in Fig. 1a. Since the entire lifetime of droplets is very long, only part of the evaporation process (100 s) is simulated. The simulation has been conducted in an axisymmetric coordinate system (see Fig. 1b).

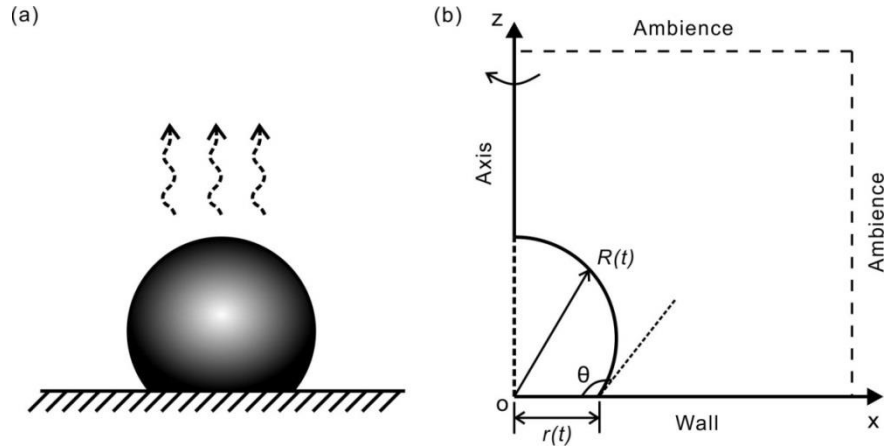


Figure 1: (a) An evaporating sessile droplet sitting on a hydrophobic substrate; (b) Illustration of a sessile droplet in the axisymmetric coordinate system.

The dimensionless squared diameters of the sessile droplets at different RH values are plotted as a function of time in Fig. 2 alongside the corresponding experimental data. It can be observed that the predictions (lines) agree well with the experiments (open markers) and each set of curve for the squared diameter shows a linear fit with time, indicating a constant change rate. Thus, the simulated process of droplet evaporation complies with the well-known “ d^2 ” law. In Fig. 2, the evaporation rate of the sessile droplet is also found to decrease with the elevated ambient humidity significantly, which reflects the inhibition of the environmental vapor on the evaporation.

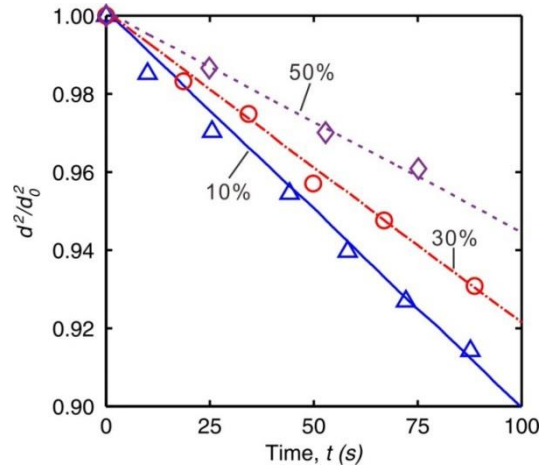


Figure 2: Comparison of numerical predictions (lines) and experimental data (open markers) [5] for the squared contact diameter of the droplet versus time.

Representative volume fractions of liquid (left) and vapor (right) for the RH of 30% are demonstrated in Fig. 3. We can see that the liquid-vapor interface in terms of the phase fractions maintains highly sharp without obvious smearing, which is ascribed to the sharp-interface scheme. A thin boundary layer of the vapor concentration is observed around the droplet and the vapor volume fraction decreases in the direction normal to the interface. Besides, the vapor tends to accumulate in the region above the droplet: The vapor concentration reaches its maximum value at the apex and minimum value near the contact line. This is ascribed to the buoyancy of the water vapor. Water vapor has smaller density than the air, and thus arises due to the buoyancy.

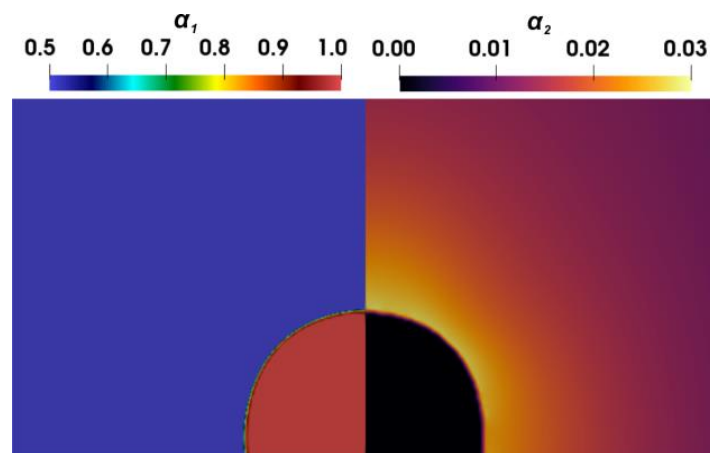


Figure 3: The simulated volume fraction fields of liquid (left) and vapor (right) at RH = 30%.

An exemplary temperature distribution at RH = 10% is presented in Fig. 4a. The droplet, especially the droplet surface depicted by the dashed line, is at a relatively lower temperature than the ambience due to the evaporative cooling effect. However, since the evaporation rate is very low, the

temperature through the computation domain is almost uniform and the maximum temperature difference is less than 1 K. The local temperature is also found to be varied along the liquid-vapor interface, with the maximum value close to the three-phase contact line and the lowest temperature at the apex. In Fig. 4b, we present the temperature profile along the axis of symmetry (i.e., z direction) extracted from Fig. 4a. The temperature declines sharply in the vicinity of the wall, indicating a thin thermal boundary layer. After a smooth decrease inside the droplet, the temperature reaches its minimum value at the interface (indicated by the dashed line) and then undergoes a steep increase in the gas phase. Due to smaller thermal conductivity, the thickness of the thermal boundary layer on the gas side is much smaller than on the liquid side. The variation of temperature clearly demonstrates how evaporation cools down the droplet and gas phase – the well-known local cooling effect of evaporation.

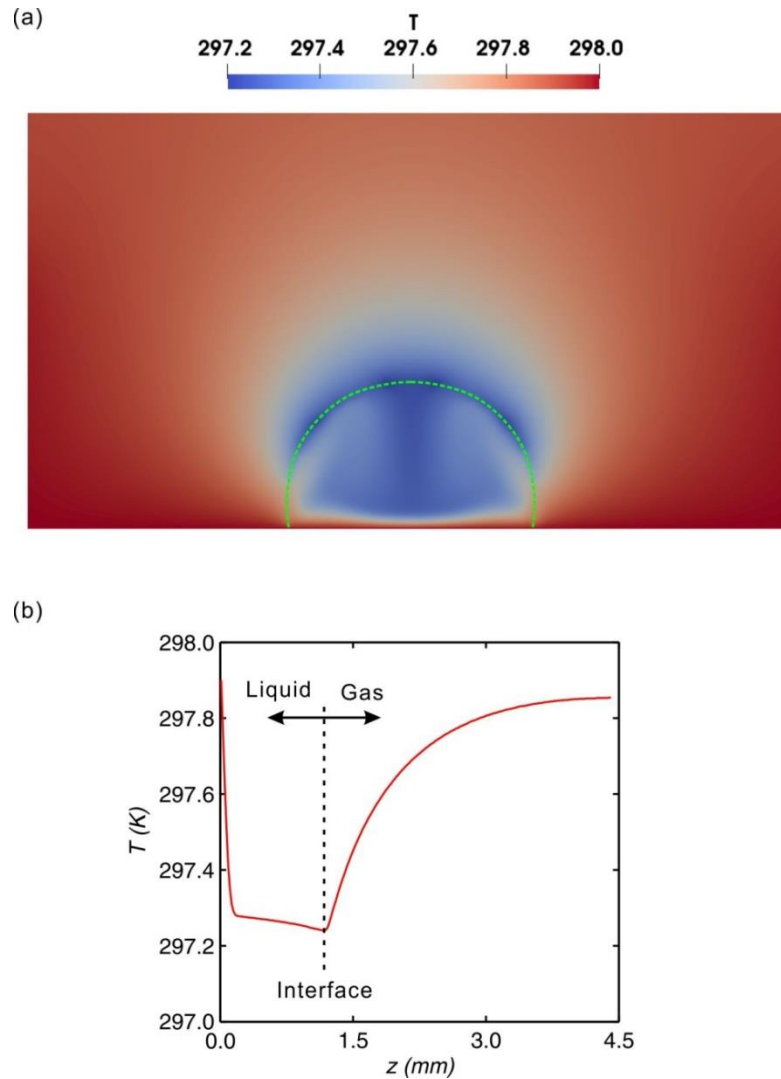


Figure 4: (a) The simulated temperature field for an evaporating sessile droplet at $RH = 10\%$; (b) The temperature profile along the axis of symmetry extracted from the temperature field in (a).

5. CONCLUSIONS

A sharp-interface algebraic VOF approach has been used for the direct numerical simulation of an evaporating sessile droplet. A specific interface identification scheme is employed to determine the explicit interface and the evaporation rate is directly derived from the local gradient of vapor mass fractions. Evaporation of a sessile droplet on a hydrophobic substrate was investigated as the case

study. Results show that the predicted evaporation rate in terms of the squared diameter agrees with experimental data at different relative humidity. The liquid-vapor interface maintains sharp without obvious smearing. The evaporative cooling mechanism at the interface is also successfully simulated. The SA-VOF approach shows great potential to predict the complex dynamics associated with droplet evaporation.

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