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On the Equations Solved for Droplet Evaporation Simulation

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Abstract

This paper presents the equations solved for the modeling of the droplet evaporation process. This model has been used to simulate the droplet evaporation process in the constant contact line phase. The validation of this model is given in Hussain et al [1]. This paper reports in detail the uses and applications of the equations used for the 2-D simulation in Hussain et al [1]. It is explained based on Ansys Fluent that was used to solve these equations.

Keywords: CFD simulation, droplet evaporation, governing equations

INTRODUCTION

The research on droplet evaporation is important in various fields of engineering and also medicine. The process of liquid droplet evaporating on a substrate can be seen in various applications such as in the creation of DNA spot arrays, in drying of paints, in cooling systems, in sprinkler systems, in spraying of pesticides and many others [2],[3],[4],[5]. Based on the need to further understand this process, various approaches have been used in studying the mechanism of droplet evaporation. This include from the use of classical methods using thermocouple probes [6] to the non-intrusive methods of using thermography [6], [7], [8] ,[9], [10], [11]. To complement the use of these experimental methods, simulations are sometimes performed when experiments are unable to provide information such as the evaporation happening inside the droplet itself. In simulating the droplet evaporation process, one needs to consider the various modes the droplet undergoes when it evaporates [12]. This paper reviews the equations that are used and solved in simulating the droplet evaporation process in the constant contact area mode.

DROPLET EVAPORATION – PHYSICAL MODEL

The physical configuration of the droplet evaporation problem is shown in Fig. 1. When a droplet is sufficiently small and surface tension force dominates over gravitational force, a liquid would take the form of a spherical cap. Based on this, the physical model adopts the spherical cap approximation which is characterized by four parameters, which are [13]:

i. the droplet height, $h(R,t)$ which is a function of the droplet radius, R and time, t.

ii. the contact line radius, R.

iii. the radius of the sphere forming the spherical cap.

iv. the contact angle between the droplet and wall, θ_W.

r and z are the radial and axial directions respectively.

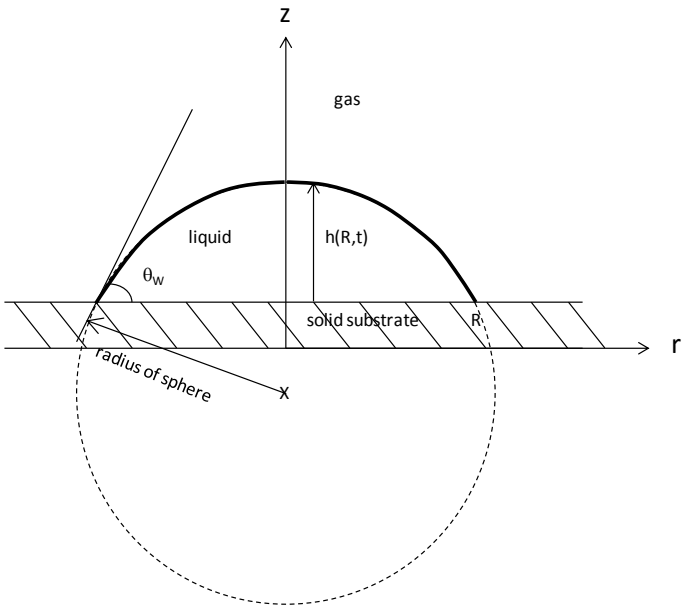

Figure 1. Physical model of the evaporation of a droplet deposited onto a substrate.

Fig. 2 shows the structure of the solution algorithm for the simulation.

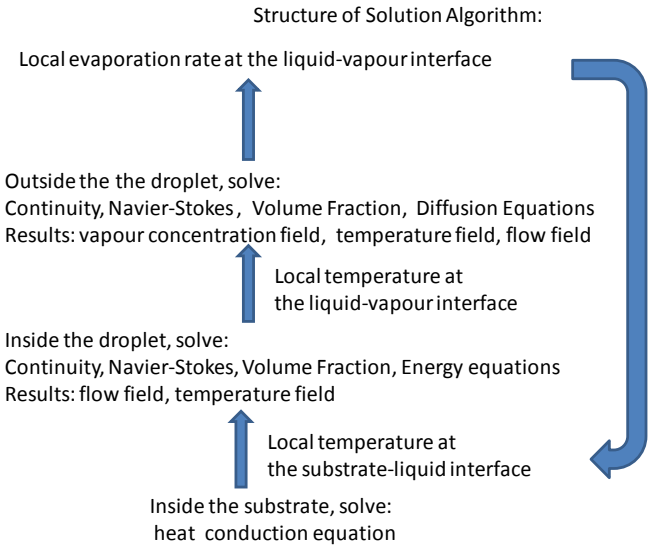

Figure 2. Structure of solution algorithm.

The following describes the equations used in the simulations. The explanation given is based on how Ansys Fluent implements the equations as described in the Ansys Fluent User Manual [14]. The equations shown are general expressions for the equations as given in the Ansys Fluent User Manual.

THE VOLUME OF FLUID (VOF) MODEL

In Ansys Fluent, there are a few models that can be used to simulate multiphase flows. There are [14]:

1. Volume-of-Fraction (VOF) model
2. Mixture model
3. Eulerian model

However, among the three, the VOF model is used for free-surface flows.

The VOF model is used for immiscible fluids, i.e. two or more fluids (or phases) which are not interpenetrating. For each additional phase that is added to the model, a variable is introduced. This variable is the volume fraction, α of the phase in the computational cell. For each control volume, the volume fractions of all the phases in the model add up to unity.

The phases share all properties and variables in the model by the volume fraction of each of the phases. For a control volume of a two-phase system with phases g and l with g being the primary phase and l the secondary phase, the properties formulation relevant to the simulation performed in this research are given in Table 1.

Table 1: Properties Formulation in Using the VOF Model

Properties	Formulation	
Density, ρ	$\rho = \alpha_l \rho_l + (1-\alpha_l)\rho_g$	(1.1)
Viscosity, μ	$\mu = \alpha_l \mu_l + (1-\alpha_l)\mu_g$	(1.2)
Thermal conductivity, k	$k = \alpha_l k_l + (1-\alpha_l)k_g$	(1.3)
Specific heat, c_p	$c_p = \frac{\alpha_l \rho_l c_{p,l} + \alpha_g \rho_g c_{p,g}}{\alpha_l \rho_l + \alpha_g \rho_g}$	(1.4)

In Ansys Fluent, the VOF model only tracks the secondary-phase [14]. Either one of the three following conditions are possible in a particular control volume for the secondary phase:

$\alpha_l = 0$: the control volume is empty of the secondary fluid or phase

$\alpha_l = 1$: the control volume is full of the secondary fluid or phase

$0 < \alpha_l < 1$: the control volume contains the interface between the secondary fluid or phase and the other fluid or phase. The volume of fraction equation is used to track the phase volume fractions in the control volume. The value of α_l in each control volume will then be used to solve for the relevant governing equations.By using the VOF model, the effects of surface tension and contact angle between the droplet and wall can be included in the simulation of the droplet evaporation.

Briones et al [15] used the explicit VOF model to model and simulate droplet evaporation. According to their paper [15], the VOF is advantageous compared to the more widely used interface-tracking methods because interface-tracking methods neglect the effect of the gas surrounding the droplets. The VOF is assumed to be able to resolve the complete physics of droplet impingement such as bubble entrapment and of droplet evaporation such as external convection. In the simulation performed by Hussain et al [1], the explicit time-marching VOF model was also used as it is a time-dependent simulation.

There are four schemes available in Fluent for calculating the fluxes in a control volume at the interface [14] which are the geometric reconstruction approach, the donor-accepter approach, the Euler explicit approach and the implicit approach. The simulation in Hussain et al [1] uses the geometric reconstruction scheme to calculate the convection and diffusion fluxes that flow through a control volume near the interface of the phases. It can be said to be the most accurate scheme between the four schemes and is flexible as it is generally used for unstructured meshes.

A. The Continuity Equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \qquad (1)$$

B. The Volume Fraction Equation [14]

As mentioned previously, the tracking of the phase volume fractions are done using the volume fraction equation:

$$\frac{\partial \alpha_l}{\partial t} + \vec{u} \cdot \nabla \alpha_l = \frac{S_{\alpha_l}}{\rho_l} \qquad (2)$$

where $\vec{u}$ is the velocity vector and ρ_l is the density of fluid or phase l. S_{α_l} is the source term in which for the case of evaporation would be the vapour generation rate.

As only the secondary fluid is tracked, the volume fraction equation is only used for the secondary fluid.

C. The Momentum Equation [14]

A single momentum equation is solved throughout the domain, and the resulting velocity field, $\vec{u}$ is shared among the phases. The momentum equation is dependent on the volume fraction of all phases through the properties of density, ρ and viscosity, μ.

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

where p is pressure. The $\vec{F}_{SV}$ is the volume force which is the force at the interface. It is a source term added to the momentum equation. It represents the effect of surface tension or the surface volume force.

The sharing of the velocity field can result in accuracy problems for the velocities near the interface if there exists a large velocity difference between the phases. There is also a possibility of convergence difficulties if the viscosity ratio is more than $1x10^3$.

D. Surface Tension, σ

During evaporation, a droplet would be dominated by either the gravity or surface tension depending on its size. For cases where the droplet size smaller than its capillary length, the droplet evaporation would be dominated by surface tension. Surface tension varies with respect to temperature. By applying a constant surface tension, the droplet shape does not become a smooth semi-spherical shape. A spherical shape is maintained by means of a correct surface tension formulation.

The surface tension model in Fluent is the continuum surface force (CSF) model by Brackbill et al [14,16]. This CSF model is implemented as a source term in the momentum equation (Equation 3) as mentioned before. The simulation considers thermocapillary-flow along the interface which occurs along the tangential direction of the interface. Hence, at the interface, the total surface force per unit interfacial area, $\vec{F}_{SA}$ is a combination of the normal surface force component, $\vec{F}_{SA}^{(n)}$ and the tangential surface force component, $\vec{F}_{SA}^{(t)}$:

$$\vec{F}_{SA} = \vec{F}_{SA}^{(n)} + \vec{F}_{SA}^{(t)} \tag{4}$$

$\vec{F}_{SA}^{(n)}$ is the force normal to the interface. It is proportional to the surface tension coefficient, σ and the curvature, κ. This is the force that drives the fluid surfaces towards a minimal energy state through a minimum surface area configuration [16].

$\vec{F}_{SA}^{(t)}$ is the force tangent to the interface that causes fluid to flow from regions of lower surface tension to regions of higher surface tension. It is due to the spatial variations of the surface tension coefficient along the interface. This is the force that results in thermocapillary-driven flows [17].

Equation 4 can be rewritten in terms of surface tension force per unit of interfacial area, $\vec{F}_{SA}$ as [17]:

$$\vec{F}_{SA} = \sigma\kappa\hat{n} + \nabla_s\sigma \tag{5}$$

where:

σ = surface tension

$\kappa = -(\nabla_s \cdot \hat{n})$ =interface curvature

$\hat{n} = \nabla\alpha_l / |\nabla\alpha_l|$ =unit vector normal to the interface pointing from the gas to the liquid

$\nabla_s = \nabla - \hat{n}(\hat{n}\cdot\nabla)$ =gradient operator tangent to the interface

For it to become a surface volume force, $\vec{F}_{SV}$ Equation 5 is multiplied with the gradient of the phase volume fraction and is rewritten as [17]:

$$\vec{F}_{SV} = (\sigma\kappa\hat{n} + \nabla_s\sigma)\cdot|\nabla\alpha_l| \tag{6}$$

This written as a surface stress boundary condition at the interface between two fluids

along the normal direction [16]:

$$p_1 - p_2 + \sigma\kappa = 2\mu_1\hat{n}_k\left(\frac{\partial u_k}{\partial n}\right)_1 - 2\mu_2\hat{n}_k\left(\frac{\partial u_k}{\partial n}\right)_2 \tag{7}$$

and along the tangential direction:

$$\mu_2\left(\hat{t}_i\frac{\partial u_i}{\partial n}\right) + \hat{n}_k\left(\frac{\partial u_k}{\partial s}\right)_2 - \mu_1\left(\hat{t}_i\frac{\partial u_i}{\partial n} + \hat{n}_k\frac{\partial u_k}{\partial s}\right)_1 = \frac{\partial\sigma}{\partial s} \tag{8}$$

where:

$\frac{\partial}{\partial s} = \hat{t}\cdot\nabla$ and $\frac{\partial}{\partial n} = \hat{n}\cdot\nabla$; $\hat{n}$ and $\hat{t}$ = unit normal and tangent respectively; μ = viscosity; u = velocity; 1 and 2 refers to the fluids 1 and 2, and i and k refers to the i_{th} and k_{th} Cartesian coordinate respectively.

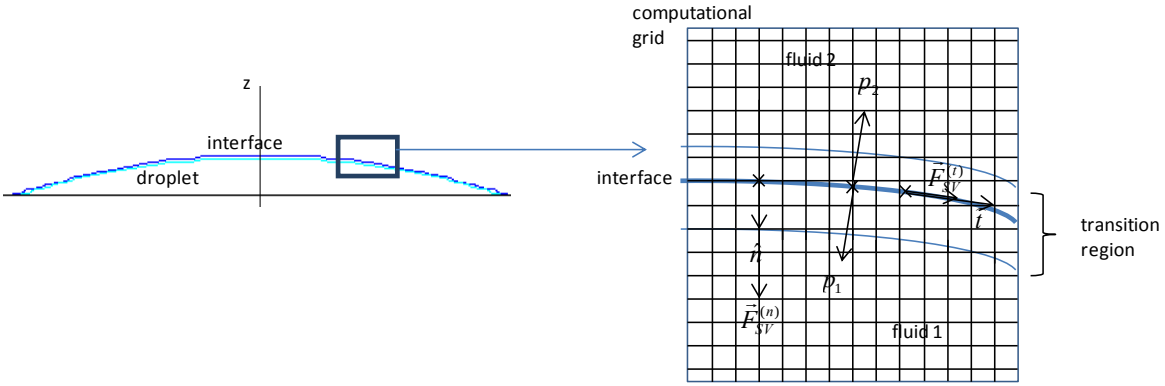

Figure 3: Surface tension formulation as explained by Brackbill et al [16].

E. ***Contact Angle Formulation***

The contact angle formulation is related to the contact dynamics of the droplet. There are a few methods that can be used to simulate contact line dynamics. Briones et al [15] outlined three strategies to simulate contact line dynamics. The first two methods are the static contact angle (SCA) and the dynamic contact angle (DCA) which utilizes the following equation [14]:

$$\hat{n} = \hat{n}_W \cos\theta_W + \hat{t}_W \sin\theta_W \tag{9}$$

where

$\hat{n}$ = the unit normal vector to the interface at the contact line between the interface and the wall

θ_W = the contact angle at the wall

$\hat{n}_W$ = the unit vector normal to the wall

$\hat{t}_W$ = the unit vector tangential to the wall

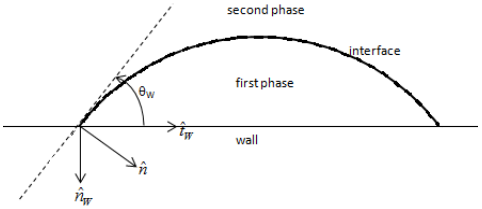

Figure 4: Contact angle representation.

In Ansys Fluent, there is an option whereby a wall adhesion angle can be specified based on the surface tension model available in the VOF model which is taken from Brackbill et al [14, 16]. From Fig. 4, it can be seen that the contact angle, θ_W is the angle between the wall and the tangent to the interface at the wall. This value is added into the simulation through the momentum equation (Equation 3) through the curvature, κ.

The SCA requires only the knowledge of the equilibrium contact angle, θ_E from the experiment where $\theta_W = \theta_E$ at all times. For the DCA, a time-dependent contact angle, θ_D needs to be obtained from the experiment; i.e. $\theta_W = \theta_D$.

The SCA option is readily available in Ansys Fluent whilst the DCA needs to be implemented through the use of a User-Defined Function (UDF) available in Ansys Fluent. This UDF is implemented through the use of a C-programming language subroutine.

The third method is Blake's contact line velocity equation [15]:

$$u_{CL} = \frac{2K_W\lambda}{\mu}\sinh\left[\frac{\sigma}{2nk_BT}\left(\cos\theta_E - \cos\theta_W\right)\right] \tag{10}$$

where

u_{CL} = the contact line velocity

n = number of absorption sites per unit area

λ = displacement length

K_W = wetting parameter

$\theta_W = \theta_D$

This model describes wetting as a dynamic absorption/desorption process of liquid molecules to the wall surface.

F. ***The Energy Equation [14]***

The energy equation is also solved through the use of a single equation used for the whole computational domain. It is also shared among the phases.

$$\frac{\partial}{\partial t}(\rho E) + \nabla\cdot\left(\vec{u}(\rho E + p)\right) = \nabla\cdot\left(k_{eff}\nabla T\right) + S_h \tag{11}$$

S_h here is the source term that is the vapour generation rate. k_{eff} is the effective thermal conductivity.

The VOF model treats the energy, E and temperature, T as mass-averaged variables. The energy for each phase is based on the specific heat of that phase and the shared temperature calculated from the energy equation.

In terms of accuracy, as with the velocity limitations in the momentum equation, a large temperature difference between the phases at the interface may lead to convergence and precision limitation.

G. ***The Diffusion Equation***

To account for the evaporation that occurs at the droplet surface, the diffusion equation is used to measure the concentration changes that occur at the interface of the droplet and its surroundings. From this measurement, the evaporation rate can be calculated. The diffusion equation is given by Fick's 2nd law. For a species q diffusing though fluid p with a constant $\rho D_{q,p}$, the diffusion equation can be written as:

$$\rho\left(\frac{\partial C_q}{\partial t} + \vec{u}\cdot\nabla C_q\right) = \rho D_{q,p}\nabla^2 C_q \tag{12}$$

where C_q is the concentration of species q. $D_{q,p}$ is the binary diffusion coefficient between the two species.

H. ***Vapour Generation Rate as Source Term***

The source term that appears in the governing equation is the vapour generation rate. The net rate of heat transfer due to heat flow is the difference between the rate of heat going in through the face area into a control volume and the rate of heat going out of the control volume across the face area plus the heat absorbed to enable phase transformation.

By application of Fourier's law of heat conduction which relates the heat flow to the local temperature gradient [18], the vapour generation rate is obtained to be:

$$\therefore \dot{m}_V = -\frac{\left[k_l(\nabla T)_l - k_g(\nabla T)_g\right]}{h_{fg}} \quad (13)$$

This $\dot{m}_V = S_{\alpha l}$ in the volume fraction equation; $\dot{m}_V = S_h$ in the energy equation; and $\dot{m}_v = S_q$ in the concentration equation.

Since a control volume is considered and the phase volume fraction determines the properties involved, the vapour generation rate is expressed as follows:

$$\dot{m}_V = -\frac{\left[k_l(\nabla\alpha\cdot\nabla T)_l - k_g(\nabla\alpha\cdot\nabla T)_g\right]}{h_{fg}} \quad (14)$$

CONCLUSION

The equations reviewed in this paper have been successful in simulating a 2-dimensional droplet evaporation process as given in Hussain et al [1]. They have also been used to simulate a 3-dimensional droplet evaporation process of which the details have yet to be published.

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