Journal of Computational Physics 340 (2017) 670–687

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Detailed finite element method modeling of evaporating multi-component droplets

Christian Diddens

Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

ARTICLE INFO

Article history:
Received 3 November 2016
Received in revised form 1 February 2017
Accepted 26 March 2017
Available online 7 April 2017

Keywords:
Droplets
Finite element method
Multi-component flow
Evaporation
Marangoni flow

ABSTRACT

The evaporation of sessile multi-component droplets is modeled with an axisymmetic finite element method. The model comprises the coupled processes of mixture evaporation, multi-component flow with composition-dependent fluid properties and thermal effects. Based on representative examples of water–glycerol and water–ethanol droplets, regular and chaotic examples of solutal Marangoni flows are discussed. Furthermore, the relevance of the substrate thickness for the evaporative cooling of volatile binary mixture droplets is pointed out. It is shown how the evaporation of the more volatile component can drastically decrease the interface temperature, so that ambient vapor of the less volatile component condenses on the droplet. Finally, results of this model are compared with corresponding results of a lubrication theory model, showing that the application of lubrication theory can cause considerable errors even for moderate contact angles of 40°.

© 2017 Elsevier Inc. All rights reserved.

1. Introduction

Evaporating sessile droplets play a crucial role in a widespread range of applications, e.g. spray cooling [1], inkjet printing [2] or biological deposition methods [3]. The improvement of these applications, e.g. the homogeneity of the deposition pattern, necessitates a thorough understanding of this ubiquitous process. A substantial contribution was achieved by Deegan et al., who were able to explain the coffee-stain effect by the enhanced evaporation rate near the contact line for droplets with a contact angle below 90° [4,5]. Based on their vapor-diffusion limited evaporation model, numerous analytical and numerical studies on drying droplets have been carried out [6–14]. However, these theoretical studies are confined to pure single-component droplets, whereas more complex droplets, i.e. multi-component mixtures, are typically used in the afore-mentioned applications.

Experimentally, it has been shown that already the addition of a second component to a sessile droplet gives rise to various remarkable effects: Due to the preferential evaporation of the more volatile component, the surface tension changes over time, which can lead to a non-monotonic evolution of the contact angle [15–21]. Furthermore, surface tension gradients along the liquid–gas interface can drive a considerable solutal Marangoni flow [22–24]. Multiple binary mixture droplets can interact through the vapor phase and can be assembled to astonishing autonomous fluidic machines [25]. By adding surfactants and polymers to a binary mixture droplet, one can overcome the coffee-stain effect and obtain homogeneous deposition patterns [26]. Finally, in ternary mixture droplets, the different volatilities and mutual solubilities of the three components can result in multiple evaporation-triggered phase transitions, as recently shown in the investigation of an evaporating ouzo droplet [27].

E-mail address: C.Diddens@tue.nl.

http://dx.doi.org/10.1016/j.jcp.2017.03.049
0021-9991/© 2017 Elsevier Inc. All rights reserved.

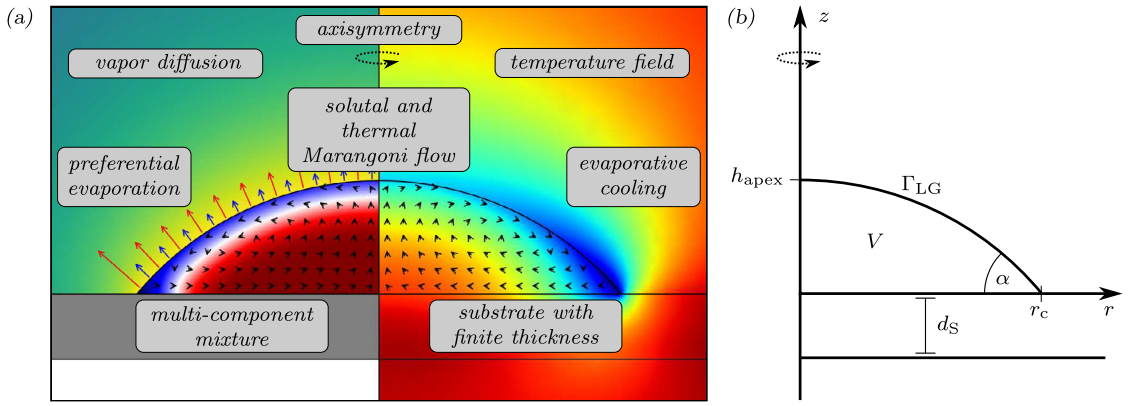

Fig. 1. (a) Schematic sketch of the considered aspects of the model. (b) Relevant geometric quantities.

From the numerical point of view, the evaporation of a sessile multi-component droplet constitutes a challenging problem, since multifarious coupled effects have to be taken into account: The evaporation rates of the individual components are coupled via the vapor–liquid equilibrium to the liquid composition and via the latent heat of evaporation to the local temperature. The mass density, dynamic viscosity, diffusivity and surface tension of the droplet are spatio-temporally varying functions of the composition and temperature as well. This can drive an in general complicated flow in the droplet, which in turn advects the composition and temperature. Temperature conduction furthermore depends on the thermal properties of the substrate.

Recently, a model for sessile multi-component droplets has been developed, which was successfully validated based on experimental data for water–ethanol droplets [28]. The same model was also able to predict the onset of oil-nucleation and the volume evolution of the ouzo droplet [27]. However, since this model is based on lubrication theory, the applicability is limited to small contact angles. Furthermore, thermal convection has been neglected.

In this study, a novel numerical model is presented, which is able to overcome these limitations by the usage of a finite element method without invoking the lubrication approximation of the Navier–Stokes equation. In section 2, the model is derived and representative results are shown and discussed in section 3. Within this context, this article focuses on the direction and regularity of solutal and thermal Marangoni flows and on the thermal influence of thin substrates. Finally, the present model is compared with the afore-mentioned lubrication approximation model. The model is successfully validated by comparing its results with experimental data in Refs. [29,30].

2. Model

The general concept of the model is depicted in Fig. 1(a): To reduce the computational effort, the model assumes axisymmetry, so that the spatial coordinates are given by cylindrical coordinates (r, z), where the substrate interface is set to $z = 0$. The substrate may have a finite thickness d_{S} with another substance below. This can be used to account for layered substrates or to investigate the thermal influence of the substrate thickness on the evaporation rate. This is discussed later on in section 3.2, where air is considered to be below the substrate.

In total, the model has to account for the coupled dynamics of multi-component evaporation, multi-component flow and thermal effects. These aspects are discussed in detail in the following sections.

2.1. Droplet shape

The droplet is assumed to be always in a spherical cap shape, i.e. the liquid–gas interface Γ_{LG} of the droplet is given by

$$\Gamma_{\mathrm{LG}}(t) = \{(r, z) \,|r \geq 0 \wedge z \geq 0 \wedge \; F_{\mathrm{LG}}(r, z, t) = 0\} \,, \tag{1}$$

where

$$F_{\mathrm{LG}}(r, z, t) = \sqrt{r^2 - \left(z - h_{\mathrm{apex}}(t) + R_{\mathrm{curv}}(t)\right)^2} - R_{\mathrm{curv}}(t) \tag{2}$$

is the implicit definition of a spherical cap with the apex height $h_{\mathrm{apex}}(t)$, i.e. the height at $r = 0$, and the radius of curvature $R_{\mathrm{curv}}(t)$ (cf. Fig. 1(b)). It is trivial to express the latter two quantities in terms of the droplet volume $V(t)$ and either the contact line radius $r_{\mathrm{c}}(t)$, defined by $F_{\mathrm{LG}}(r_{\mathrm{c}}(t), 0, t) = 0$, or the contact angle $\alpha(t)$. Therefore, the droplet shape $\Gamma_{\mathrm{LG}}(t)$ is entirely defined by its current volume $V(t)$ and r_{c} in case of a pinned contact line, or by $V(t)$ and $\alpha(t)$ in case of an unpinned contact line. Of course, this can easily be generalized to stick-slip motions as well. The benefit of defining Γ_{LG} in the implicit manner (1) is the possibility to allow for contact angles $\alpha > 90°$.

Download English Version:

https://daneshyari.com/en/article/4967310

Download Persian Version:

https://daneshyari.com/article/4967310

Daneshyari.com