International Journal of Heat and Mass Transfer 105 (2017) 655–663

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Experimental and numerical investigation of drop evaporation depending on the shape of the liquid/gas interface

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ARTICLE INFO

Article history:
Received 1 June 2016
Received in revised form 23 September 2016
Accepted 8 October 2016

Keywords:
Water drop evaporation
Phase field model
Computer simulation
Experimental study
Interface shape

ABSTRACT

We present experimental and numerical lifetime investigations of evaporating water drops on solid surfaces depending on the shape and size of their liquid/gas interface. The simulations are based on an Allen–Cahn type phase-field model, where the liquid–gas phase transition is driven by a concentration gradient. The experiments are conducted under defined initial and constant conditions. Throughout the whole experiment, contact angle, temperature, relative air humidity and drop weight are tracked continuously. The numerical and experimental results are compared with analytical predictions. In our study, we confirm that the lifetime of a drop is directly linked to its surface size and shape. We compare lifetimes of evaporating drops on smooth solid surfaces with different contact angles and find an increase in lifetime by 50% as the contact angle increases from 20° to 90°, both in experiments and in simulations. Furthermore, drops placed in different geometric set-ups such as a wedge or a corner show a lifetime behavior that is in accordance with analytical predictions. The presented computational approach captures experimentally measured drop lifetimes, for various set-ups, very well. These findings are especially relevant for industrial questions such as how fast complex components dry after cleaning or how long it takes till lacquer layers are cured on structured surfaces.

1. Introduction

Since decades, scientists are concerned with the evaporation of small liquid drops on flat surfaces [1,2]. In industry though, the need for knowledge about the evaporation process of drops on structured surfaces or in gaps is increasing due to the urge of perfectly timed production lines. In order to know the exact time that a technical component needs to dry before further processing, it is necessary to understand the evaporation process of drops on 3D geometries. As well as for the cleaning processes this knowledge is useful to predict the drying time of lacquer layers on structured surfaces.

Cazabat and Guéna [3] presented a review article on the evaporation of macroscopic sessile drops in normal atmosphere from the point of view of experimentalists. Beside experimental results, they introduce analytical solutions for specific evaporation processes. Erbil [4] presents a review including a comprehensive range of published articles on the evaporation of sessile drops and nearly spherical drops. The basic theory of the evaporation of micro and millimeter sized spherical droplets and drops on super hydrophobic surfaces is widely discussed. Moreover, the author reports the effect of contact angle hysteresis, substrate thermal conductivity and Marangoni flows on the evaporation process. Recent works compare two commonly used evaporation models with respect to the evolution of the drop radius during evaporation [5] and show the influence of contact angles on droplet lifetimes for a wide range of initial contact angles [6]. The analytical derivation describes the dependence of droplet lifetime from the initial contact angle as well as from its hysteresis.

Experimental studies are also concerned with the influence of the contact angle on evaporation rates. Chandra [7] for example, experimentally reports that evaporating droplets of 0, 100 and 1000 ppm surfactant solutions show a lifetime decrease of 50% by changing the contact angle from 90° to 20°. This observation underlines the effect of the surface shape and size on the evaporation rate. The same trend is observed by Kulinich [8], who states an increase in evaporation rate due to pinning. A good description of the evaporation modes of weakly and strongly pinning surfaces is given by Bormaschenko [9]. He experimentally verifies the model describing stick–slip motion of evaporating droplets presented by Shanahan and Sefiane [10]. Javadi et al. [11] discuss experimental

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2016.10.033
0017-9310/

and numerical results showing how two drops shrink and grow due to their wetting angle and surface curvature in small closed systems.

Moreover, in the last two decades, a wide range of simulation models related to evaporation phenomena were introduced. While early approaches with Molecular Dynamics simulations [12,13] are restricted to very small volumes, phase-field models (PFM) become more and more the tool of choice for the simulation of evaporating micro and millimeter sized droplets. Borcia and Bestehorn [14] formulate an extension of PFM [15] by an additional temperature gradient dependent contribution and investigate the influence of thermal Marangoni convection on the evaporation behavior of a liquid–vapor system, by coupling the PFM to a Navier–Stokes model. Badillo [16] develops a phase-field approach based on a modified Cahn–Hilliard model, coupled to heat and fluid flow equations. The model accounts for phase changes and surface tension effects at the liquid/gas interface, of pure substances with large property contrast, induced by temperature gradients. Numerical computations illustrate a good agreement with analytical as well as experimental results. Ledesma-Aguilar et al. [17] and Safari et al. [18] presented phase-field lattice-Boltzmann models, where the liquid/gas phase transformation takes place due to concentration gradients. Dietrich et al. [19] recently presented an experimental study showing the importance of convection for drop evaporation. They stated that convection plays an important role for Rayleigh numbers larger than 12. Using this correlation Laghezza et al. [20] discussed the influence of convection on the dissolution process of various droplet patterns. They found that enhanced convection above droplet patterns can reduce the dissolution time of droplets at the edges of the pattern to values below that of a single, isolated droplet. The presented results deal with flat or perfectly axis-symmetric droplets. However, in a wide range of industrial applications arbitrary surfaces and droplet sizes, where gravity forces cannot be neglected, are especially interesting. Thus, the current work is focused on the following question: How does the lifetime or equilibrium shape of drops change depending on their surface shapes? The surface shape of a drop is varied by (i) placing the drop on three different substrate geometries and (ii) changing the contact angles between the liquid and solid phase. Hence, we focus the investigation on the lifetime (in open systems) and the equilibrium state (in closed systems) of a drop on a solid surface. We present a PFM of Allen–Cahn type, where the liquid/gas phase transformation takes place due to a difference in saturation concentration and local partial concentration. For the proposed phase-field model the kinetic coefficient τ is calibrated by comparison with experimental data. The determined coefficient is used for all other geometrical settings and well recovers the experimental diffusion and evaporation behavior.

In Section 2, we introduce the experimental set-up, before we explain the PFM in Section 3. Here, assumptions are explained and an energy density contribution $f_{evap}(\phi)$, reflecting evaporation effects, is introduced. Then, we present the test set-up for the experimental study as well as the simulations in Section 4. The results are compared and discussed in Section 5 for an open system (constant partial pressure) and in Section 6 for a closed system where the partial pressure increases till the saturation pressure of the system is reached. Finally, in Section 7 we present our conclusions.

2. Experimental set-up

In this section the experimental set-up for drop observation is introduced. Over time, the contact angle, the mass of the drop and relative air humidity and temperature are tracked. In the case of an open system, the set-up is placed into an airtight glove box of 0.5 m^3, see Fig. 1. Herewith it is possible to establish constant conditions such as relative air humidity and still air. The glove box is large enough to ensure that the amount of water evaporating from the drop does not influence the initial relative air humidity. As closed system, an airtight container of 250 ml is used. Since, in this case, the focus is on a saturated gas phase, the system volume is small enough to saturate without a significant change in drop volume. In order to track the mass loss of drops over time, the substrates are placed on a lab scale that is connected to a computer. To measure the contact angle throughout the whole evaporation process, drop images are taken every five minutes.

Fig. 1 displays a schematic experimental set-up for an open system. The surrounding line corresponds to the system boundary, in this case the glove box. Using an Eppendorf pipette drops are placed on different substrates. The weight loss is tracked with a Mettler Toledo AX105-DR lab scale with a measurement precision of ±0.01 mg. A camera 2250 M from IDS Imaging takes pictures of the drop shape, to analyze the contact angle with the Krüss software DSA II. Pictures are stored by the free-ware software yawcam. To ensure a black drop scheme in front of a bright background, a light source KL1500 from Schott stands on the opposite side of the drop outside the box. Additionally, a diffuser is placed in front of the light to ensure an homogeneous background. Furthermore, temperature and relative air humidity are measured during the whole evaporation process using four SHT21 sensors from Sensirion (measurement precision ±3%). These are placed in different corners of the glove box and one close to the evaporating drop. To ensure constant relative air humidity, RH, at different levels, saturated salt solutions of Sodium hydroxide (NaOH), Magnesium chloride (MgCl$_2$) and Potassium iodide (KI) in large flat bowls are integrated into the set-up, see Table 1.

For the closed system, drops are placed on substrates within the airtight containers in front of the camera. The air humidity is measured by a data logger included in the container. Due to the small size of the system, it is experimentally not feasible to track the weight of the liquid drops. Results are obtained through optical measurements only.

3. Simulation methods

When a water drop evaporates from a substrate, its volume decreases in time and its shape changes in order to form an ener-

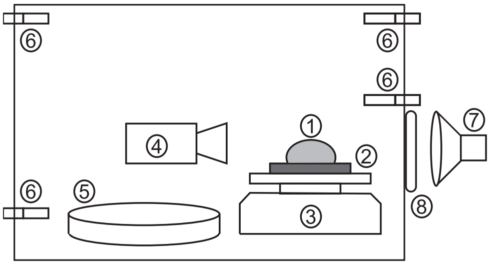

Fig. 1. Experimental set-up; (1) drop, (2) substrate, (3) lab scale, (4) camera, (5) bowl with saturated salt solution, (6) humidity/temperature sensors, (7) light source, (8) diffuse layer.

Table 1
Salts to vary the relative air humidity in the experiments (measured values including maximal deviations).

Salt	RH at 295 K	Max. dev.
Sodium hydroxide	17%	±2%
Magnesium chloride	37%	±2%
Potassium iodide	65%	±3%