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One-dimensional models of nanoliter droplet evaporation from a hot surface in the transition regime

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ABSTRACT

A novel one-dimensional model of the evaporation of liquid water droplets from a hot surface is presented. The one-dimensional finite-difference model solves the governing equations of continuity, momentum, species and energy within the gaseous phase in spherical coordinates. The model includes the Hertz–Knudsen kinetic evaporative mass flux with a correction for the transitional regime that exists between continuum and molecular length-scales. The accommodation coefficient of the kinetic mass flux is constant and set to unity while the droplet thermal conductance is a multiple of the thermal conductivity of water. The model employs a uniform discretization of the spherical vapor region surrounding the droplet and a one-dimensional conduction model of the droplet itself. The model can also emulate pinned and de-pinned contact lines based on a geometric expression. Several theories of evaporative mass flux in the transition regime are compared. Droplet evaporation data is acquired with a standard dispensing/imaging system and high-speed photography. The calculated, transient droplet volumes are compared to experimental evaporation data of sessile droplets ranging from 30 to 80 μm initial radius (0.06–1.4 nanoliters). Simplification of the one-dimensional equations leads to a semi-analytical model. Good agreement is achieved between both models and the experimental data. Results indicate that the evaporation process is a greater resistance to overall heat transfer than conduction through the droplet itself, which is consistent with the previous results of axisymmetric volume-of-fluid (VOF) models.

1. Introduction

Spray and thin-film cooling technologies are used in a variety of industrial applications such as microelectronics [1], transportation [2], metal production and processing [3,4], and surgical laser equipment [5]. These cooling methods are important to industry because of their ability to uniformly remove large heat fluxes while only requiring a small volume of fluid [6]. Also, isothermal temperature control can be accomplished by exploiting the large heat of vaporization of the working fluid.

The study of spray cooling in a full-scale application is difficult due to the large number of droplets that would have to be modeled and tracked as well as the complex fluid dynamics present. These processes involve the formation of a droplet spray with a distribution of droplet sizes that may also interact with one another upon impingement with the surface. Impact of the droplets on a surface can result in droplet deposition, spreading, recoiling, jetting, and rebound, for example. These processes may be followed by droplet pinning and inertial oscillations that are subsequently followed by evaporation. During the evaporation process the droplet could remain pinned or de-pin depending on circumstances such as the surface temperature, surface geometry, roughness, and hydrophobicity.

To remove many of the complexities in spray cooling that are a barrier to fundamental understanding, studies are often performed on single droplets. When impinging on a surface, droplets undergo a transient deformation process from a spherical shape to a spherical cap. The short-time droplet impact dynamics can be de-coupled from the evaporation process due to the several orders of magnitude difference in their time scales [7]; for a 50 μm diameter droplet, the impact dynamics subside at around 100 μs while the evaporation takes around 100 ms. In addition, the amount of heat removed by a droplet during the short-time impact dynamics is insignificant. Once the droplet has evolved into a spherical cap shape, it will start to decrease in volume due to the evaporative mass flux from the liquid–gas interface to the surroundings. This transient process is driven by conditions at the interface and the saturation ratio of the gas mixture. Also, as the droplet volume decreases, the contact line could de-pin (or recede). It may remain pinned to the surface at a specific absorption site until the unbalanced Young–Laplace force causes motion [8].

There is vast literature on experimental and numerical investigations of single droplet evaporation. Both molecular dynamics (MD) and computational fluid dynamics (CFD) simulations are

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Nomenclature

Latin

A	surface area
c	molecular velocity, specific heat
C	constant from continuity solution
D_{ab}	binary diffusion coefficient
E	internal energy per unit volume
h_{fg}	enthalpy of vaporization
k	thermal conductivity
Kn	Knudsen number
L	droplet height
m	mass
$\mathcal{M}$	molecular mass
p	pressure
q	heat
r	radial coordinate, contact radius
R	radius of curvature, specific gas constant
$\mathcal{R}$	universal gas constant
t	time
T	temperature
V	volume
z	ratio of molecular masses

Greek

β	modified accommodation coefficient
γ	molecular reflection parameter
λ	mean free path
μ	absolute viscosity
ρ	density
σ	accommodation coefficient
ω	mass fraction
θ	contact angle
Δ	Knudsen layer thickness

subscripts

a	air species
c	contact line
kin	kinetic theory
l	liquid
lv	liquid–vapor
v	vapor species
w	wall

superscripts

$''$	flux (per unit time per unit area)
$\bar{}$	mean
$\dot{}$	rate (per unit time)

fairly abundant in this area of research [9]. With MD simulations, high computational bandwidth is required and only a small fraction of real-time behavior is tractable to simulate. However, several researchers have used this method to compute values of the accommodation coefficient [10–12]. Regarding CFD investigations, there are two mainstream methods: interface-tracking [13] and interface-capturing [14,15]. However, both interface-tracking and interface-capturing computational methods are tremendously stiff due to the inherent Marangoni time scales. The total simulation time for sessile droplet evaporation using adaptive mesh refinement can approach 4–6 weeks.

In this investigation, we formulate a one-dimensional finite difference method to avoid the higher-order complexities of the computationally-expensive, high resolution interface-tracking and interface-capturing methods. The model neglects internal and external convection; the droplet conducts heat from the surface to the liquid–vapor interface, and the gas mixture transports heat and mass through advection and diffusion. The model can represent either pinned or de-pinned droplet geometry. Further simplification of the numerical model leads to a semi-analytical model. These numerical and analytical models can be used for comparison of transient volume profiles of a large number of droplet parameters, such as accommodation coefficient, droplet thermal conductivity, density, specific heat capacity, viscosity, and molecular mean free path, as well as to compare various evaporation mass flux theories in short times unattainable by CFD simulations. These one-dimensional models are important to assess the efficacy of coolants based on their thermodynamic and transport properties. Other one-dimensional models exist. For example, Shedd [16] calculated bubble dissolution and droplet evaporation times by numerically integrating rate equations based on empirical mass transfer coefficients. While this greatly simplifies the model, it is based on continuum theory and not entirely applicable to the current problem.

In the current work, the droplet radii of interest are tens to hundreds of microns; this corresponds to nanoliter and below volumes. The surface temperatures are held below the boiling point. The evaporative mass and heat fluxes occur within the so-called transition regime, which is bounded by continuum theory for relatively large droplets and kinetic theory for very small droplets; this theory is detailed in the next section. Kulmala [17] examined both continuum theory and a transitional regime correction to the continuum theory to derive an analytical expression for the evaporation time of spherical droplets. First order expansions of the mass flux were employed in order to develop an expression that was integrated over time. Only the liquid phase was modeled with continuum theory equations. Hu and Larson [18] compared both analytical and computational techniques against experimental sessile droplet evaporation data. Their analytical expression modeled a pinned cap-shape droplet under the action of continuum theory evaporation; the surrounding gas was not modeled and the interface temperature was constant. In contrast, the present work employs transitional regime corrections to the kinetic mass flux and uses continuum transport equations in the gas phase for both pinned and de-pinned (near hemispherical) micro-droplets.

While the motivation for modeling heat and mass transfer of micro-droplets is to gain technical confidence and competence in the understanding of spray and thin film cooling, the intent of this investigation is to understand droplet evaporation for micro-droplets with initial radii of 30–80 μm. The specific objectives of this research are to: (1) develop a one-dimensional finite difference model for sessile droplet evaporation for both pinned and de-pinned modes, (2) develop a one-dimensional semi-analytical model for sessile droplet evaporation, (3) compare various evaporation flux transition models as function of droplet radius, (4) validate the simulations against measured, transient volume and contact radius data for various micro-droplets, and (5) compare the numerical and semi-analytical models.

2. Evaporative flux model

The most important component of the droplet evaporation model is the calculation of the evaporative mass and heat fluxes from the liquid phase to the gas phase. This section provides a brief review of several different expressions for these.