A Fully Coupled Time Dependent 3-D Axisymmetric Simulation of an Evaporating Sessile Drop

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Abstract

Drying a droplet of a colloidal suspension is a simple method to deposit particles on solid surfaces. Different deposition patterns can be obtained depending on several aspects such as, the evaporation mechanisms, solid substrate-liquid interactions, and colloidal particle concentrations. There are interests in understanding the fluid dynamics during evaporation of the solvent in order to control the distribution of the deposited particles. Studies have been done analytically and numerically with different types of evaporation fluxes at the droplet interface to determine the effect of these fluxes on the fluid flow profile in the droplet. These studies have been done mostly on small droplets where the gravitational force is negligible.

The Navier-Stokes system of equations are solved numerically in order to understand the time dependent dynamics inside an evaporating sessile droplet. The nonlinear, time-dependent governing equations are solved numerically by using the Galerkin/finite element method (G/FEM) for discretization of the spatial domain and an adaptive finite difference method for discretization in the time domain. The droplet shape, and velocity and pressure profiles inside the droplet are solved simultaneously. The algorithm has been successfully applied to study sessile drop evaporation where the inertial force can be important (Reynold numbers is not low) and where the gravitational force is absent or present. Currently, a uniform and constant evaporation flux is imposed through the kinematic boundary condition. The next step is to solve simultaneously the Navier-Stokes equations which govern the fluid dynamics inside the droplet and the Laplace equation which govern the vapor concentration outside the droplet. The evaporation flux will be calculated from the vapor concentration gradient.

Introduction

The focus of this study is the numerical study of the fluid dynamics inside an evaporating pure liquid sessile droplet. The nonlinear, time-dependent governing equations are solved numerically by using the Galerkin/finite element method (G/FEM) (Strang & Fix, 1973) for discretization of the spatial domain and an adaptive finite difference method for discretization in the time domain.

The motivation behind this study is to understand the effect of the fluid dynamics inside an evaporating droplet on the distribution and the arrangement of the particles deposited on the substrate prior to evaporation. Studies had been done on the flow profile during an evaporation of small or thin droplets at low capillary and Reynolds numbers with negligible gravitational forces. Studies need to be done on more general cases where the inertial force can be important and where the gravitational force is absent or present.

Researchers have investigated the relation between flow profile inside the drying sessile droplet and the particle distribution on the substrate after drying, experimentally and numerically. Deegan et al. (1997) investigated the evaporation of a droplet containing a suspension of colloidal particles. During evaporation, the droplet contact line was fixed, which resulted in an outward flow carrying the particles to the perimeter of the droplet, and a ring of particles was formed.

Fischer (2002) examined the drying of very thin droplets with pinned contact lines and negligible gravitational terms. Three different evaporation flux cases were considered: uniform flux across the droplet interface, non uniform flux varying from the largest flux at the center of the droplet to the smallest flux at the edge of the droplet and non uniform flux varying from the smallest at the center to the greatest at the edge. He used the lubrication approximation to simplify the governing equations. Drop height profile, the flow profile and the particle distribution profile were solved for each evaporation model.

Hu and Larson (2005) solved the flow field inside an evaporating sessile droplet analytically using lubrication approximation and verified the result numerically using finite element method. He considered a small droplet with a pinned contact line without gravitational force; hence the drop shape was a section of a sphere. The numerical and the analytical flow profile results agree very well for a droplet with small contact angles.

Liu (1999) and Li (2001) solved the Navier-Stokes system to obtain the flow dynamics inside an evaporating sessile droplet with a fixed contact line. Two-dimensional time-dependent flow and shape profiles were obtained by solving numerically the equations of motion using the Galerkin/finite element method. The mesh was generated using the spine method. The equations were integrated in time with an implicit time integration scheme using a fixed time step size.

In this study, Liu's and Li's works on evaporating pure liquid drops are replicated. An adaptive implicit time stepping is implemented to integrate the equations in time. One variation from previous studies is the division of the drop domain into three subdomains. One subdomain covers the area close to the free surface, another one covers the area close to the substrate, and another one covers the rest of the area. Each subdomain has a different mesh resolution.

The utilization of the spine mesh method in discretizing a highly curved free surface problem can also be seen in studies by Notz and Basaran (1999) and Wilkes, et al. (1999). In both works, the spine method was used to discretize the spatial domain of a pendant drop hanging on a nozzle. Because of the highly deformed and elongated drop shapes can be obtained, the physical drop domain was divided into several subdomains. Remeshing method was adopted in order to capture information on the drop neck region, close to the breakup time.

Problem Formulation

In this work, a Galerkin finite element method is used to solve numerically the velocity field, pressure field and the shape of the droplet during evaporation. The system is an axisymmetric sessile droplet of an incompressible, Newtonian liquid of spatially uniform and constant viscosity (μ) and density (ρ). The aspect ratio of the droplet is obtained by dividing the height of the drop (h) by the fixed radius at the contact line (R). The ambient fluid, which is air, exerts a uniform pressure and negligible viscous drag on the droplet. The surface tension (σ) of the liquid-gas interface is spatially uniform and constant. No temperature gradient is assumed here. The gravity **g** is acting downward.

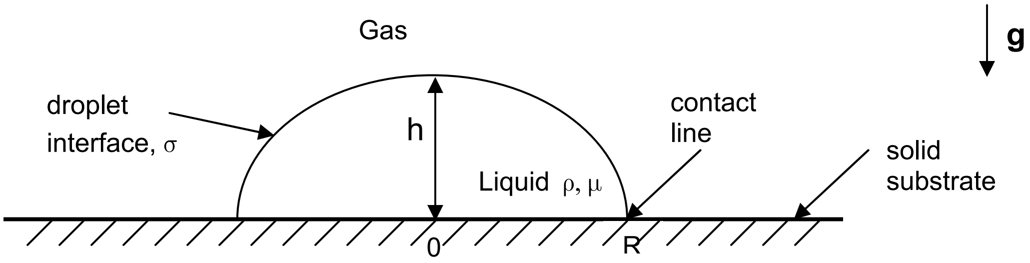


Fig. 1. Axisymmetric sessile droplet with radius R

Initially, the sessile droplet is sitting on a solid substrate at its equilibrium configuration, determined from solution of the Young-Laplace equation. In the absence of the gravitational field, a hemispherical shaped droplet is obtained. After the equilibrium configuration is attained, a constant and uniform evaporation flux ($\tilde{J}$**)** is imposed along the free surface. The contact line is fixed throughout the evaporation process.

Result

The dynamics of sessile droplet evaporation has been solved numerically using Galerkin finite element method (G/FEM). As the droplet is evaporating, the height and the contact angle of the drop decrease. At the end of the evaporation time, a thin droplet remains. The droplet shape, and velocity and pressure profiles inside the droplet are solved simultaneously.

Two ways of discretizing the physical drop domain are illustrated in Fig. 2. As the drop evaporates, the contact angle decreases which causes the element at the contact point to become distorted. When the element at the contact line becomes extremely distorted, the algorithm fails to converge. For the element discretization shown in Fig. 2a, the algorithm does not work well at small aspect ratio, because the element at the contact line is too coarse. For the element discretization shown in Fig. 2b, the algorithm works well at small and large aspect ratio. By refining the elements close to the contact line the distortion of the element at the contact point is distributed, minimizing the local distortion.

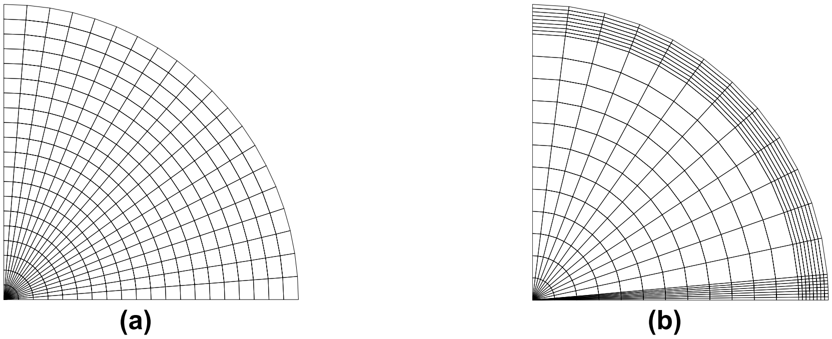
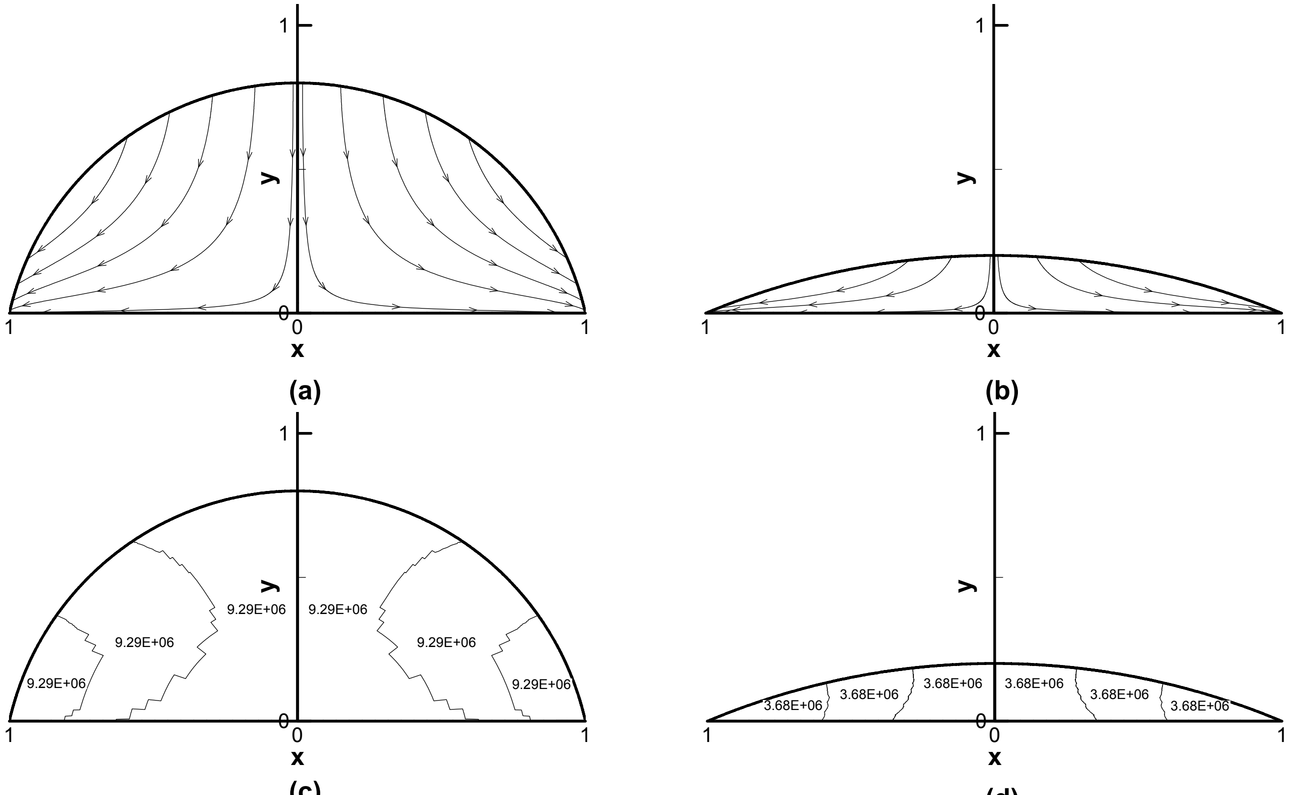


Fig. 2. Droplet physical domain discretization using a)one region, b)three regions.

Fig. 3 shows the streamline profile and the pressure profile inside an evaporating droplet at different point of time for the mesh discretization shown on Fig. 2b. The velocity in the negative y direction is dominating very close to the symmetry line, and the velocity in x direction is dominating very close to the solid substrate. The fluid is flowing outward in order to replace the evaporated solvent while fixing the contact line. The pressure is uniform inside the droplet.



(a) (b) (c) (d)

Fig. 3. The streamline inside an evaporating droplet at, a)time = 0.1, b)time = 0.4. The pressure inside an evaporating droplet at, c)time = 0.1 , d)time = 0.4.

5. Conclusions

The fluid dynamics inside an evaporating sessile droplet with a pinned contact line has been solved numerically. The droplet shape and velocity and pressure profile inside the droplet are solved simultaneously. The algorithm can be applied to study sessile drop evaporation where the inertial force can be important (Reynold numbers is not low) and where the gravitational force is absent or present (Widjaja, et al., 2005). Currently, the focus of the study is to include the Laplace equation which govern the vapor concentration outside the droplet. The evaporation flux will be calculated from the vapor concentration gradient.

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