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# Numerical simulation of the drying of inkjet-printed droplets

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## ARTICLE INFO

### ABSTRACT

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Keywords: Fluid dynamics Evaporation Adsorption Droplet Spreading In this paper we study the behavior of an inkjet-printed droplet of a solute dissolved in a solvent on a solid horizontal surface by numerical simulation. An extended model for drying of a droplet and the final distribution of the solute on an impermeable substrate is proposed. The model extends the work by Deegan, Fischer and Kuerten by taking into account convection, diffusion and adsorption of the solute in order to describe more accurately the surface coverage on the substrate. A spherically shaped droplet is considered such that the model can be formulated as an axially symmetric problem. The droplet dynamics is driven by the combined action of surface tension and evaporation. The fluid flow in the droplet is modeled by the Navier–Stokes equation and the continuity equation, where the lubrication approximation is applied. The rate of evaporation is determined by the distribution of vapor pressure in the air surrounding the droplet. Numerical results are compared with experimental results for droplets of various sizes.

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#### 1. Introduction

For many industrial applications, inkjet printing is an important field of research. Examples of application areas are printing of ink on paper and printing DNA or protein molecules solved in a buffer fluid on microarray slides. The formulation of biomolecule solutions that give well-controlled 3D highly functional bio-layers after drying is regarded as one of the main challenges in the worldwide microarray community [1].

Microarray manufacturing starts by spotting the protein samples onto a flat horizontal surface using an inkjet printer. After the droplet collides with the surface, its kinetic energy will cause spreading and shrinking until it reaches an equilibrium shape [1– 3]. The time scale from the impact to the equilibrium shape is small compared to the typical time of evaporation, which, depending on humidity and temperature, takes several seconds. Hence, the impact and the evaporation of the droplet can be separated into two independent processes.

During the evaporation phase, the dynamics of the fluid drives the protein molecules and a thin layer of deposit on the surface is formed that is partly bound to the substrate after total evaporation of the solvent. The way in which the biomolecules bind to the surface determines the functionality of the microarray [4].

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Therefore, the evaporation process plays an important role in the quality of the microarray [5].

The mass transfer resulting from evaporation causes a change in the shape of the droplet. The evaporation of a sessile droplet can take place in two different ways: either the contact line moves while the contact angle remains constant, or the contact line is pinned while the contact angle decreases [6–8]. A mixed situation with a stick–slip motion of receding contact angle is also reported in literature [9]. This especially can occur during the final stages of the evaporation process. Which of the two ways of evaporation takes place depends on many parameters, for instance the hydrophobicity of the substrate, the rate of evaporation and the surface roughness.

The first model for dewetting, proposed by Young, describes the contact angle in terms of the interface tensions between air, liquid and the solid substrate. Since then, numerous studies have been conducted in order to relate the contact line behavior to the properties of the substrate. In their paper, Shin et al. [10] concluded that in the evaporation of a sessile droplet on a hydrophobic surface, in which the initial contact angle is considerable, the contact line has a higher tendency to recede. In contrast, Golovko et al. [11] determined from experiments that for a droplet with a smaller contact angle, the contact line tends to be pinned during the evaporation process. This result is supported by experimental research by Bourges-Monnier and Shanahan [12], who observed that for a contact angle smaller than 90°, the contact line is anchored during the evaporation.

One of the earliest contributions to the understanding of the dynamics of the solvent and solute was made by Deegan et al.

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[13–15]. They assumed that the surface is so inhomogeneous that the contact line remains pinned during evaporation of the droplet. A pinned contact line is only possible if the evaporation in the area close to the contact line is compensated by convection from the center of the droplet to the edge. This process leads to the wellknown coffee stain effect. An extension to this model was made by Fischer [16], who did not assume the shape of the droplet to be spherical during the evaporation process. Instead, he proposed a dynamic shape depending on the evaporation rate along the surface area. Van Dam and Kuerten [17] proposed an extension for the calculation of the curvature of the droplet shape in order to account for a droplet with a larger contact angle and considered a concentration-dependent viscosity of the liquid inside the droplet.

The singularity at the contact line is the main obstacle to model the dewetting process. The no-slip boundary condition at the liquid–substrate interface contradicts the fact that the contact line recedes with a certain velocity. This is known as the Huh and Scriven paradox [18]. One way to circumvent this singularity is by introducing slip along a small distance from the contact line which is quantified by the slip length [19–21]. Another way to solve this paradox is to use the concept of a submicroscopic precursor film [22,23]. In this approach, a thin film is assumed to cover the dry area outside the wetting area. Hence, the contact line is defined on the surface of the precursor film where fluid velocity (also called slip) is possible. In order to ensure equilibrium at the contact line, Schwartz and Eley [24] propose a model for disjoining pressure based on the Frumkin–Deryugin model, which describes the interaction between molecules.

Protein adsorption is a complex, dynamic process which involves noncovalent interactions, including hydrophobic interactions, electrostatic forces, hydrogen bonding, and van der Waals forces [25]. This process is mainly affected by the properties of the surface, the nature of the protein and the solution condition [26]. One of the earliest kinetic models is derived from the classical Langmuir equation for gas adsorption [27]. This model describes the adsorption process in the equilibrium state, by assuming that the adsorption is a purely reversible process. In later work by Lundström and McOueen [28]. Beisinger and Leonard [29] and Soderquist and Walton [30], the classical steady-state Langmuir model is extended to a time-dependent model by including more complex physical phenomena such as resorption and reversible adsorption. However, validation of these models only gives a qualitative agreement with experimental results [31]. Kurat et al. developed an adsorption model for bovine serum albumin at silica-titania surfaces [32,33]. They showed that their theoretical model is in good agreement with their experimental results.

In this paper, we present a numerical method for the fluid dynamics and the motion and final deposition of solute molecules during the evaporation of an inkjet-printed droplet on a solid substrate. The method is based on models for flow of the liquid, convection and diffusion of the solute and binding of the solute molecules to the substrate. We will compare results of the model with experimental results for droplets of various sizes and perform a sensitivity study by varying the most important physical parameters in the models.

#### 2. Mathematical models

The mathematical model covers the dynamics of the solvent due to evaporation, the concentration of the solute and the binding of the solute molecules to the surface. We consider two separate cases for the contact line dynamics: a pinned and an unpinned contact line. As we consider dilute solutions we neglect the influence of concentration on viscosity. Fig. 1 depicts an axially symmetric droplet (a spherical cap) on a horizontal substrate with *H* and *R* the initial height and radius respectively, and  $\theta_c$  the contact angle.



Fig. 1. Sketch of a spherical droplet on an impermeable substrate.

#### 2.1. Lubrication equation

A complete model for the flow inside the droplet is provided by the three-dimensional Navier-Stokes equation and the continuity equation for an incompressible fluid. However, a study of the order of the magnitude of the terms in these equations reveals that the model can be simplified by the lubrication approximation. Moreover, only situations with cylindrical symmetry, in which the quantities do not depend on the azimuthal coordinate and the azimuthal velocity equals zero, will be considered. The most important assumptions in this simplified model are that the height of the droplet is much smaller than its radius and that the height of the drop is well below the capillary length. The capillary length is defined as  $l_{\sigma} = (\sigma/\rho g)^{1/2}$ , where  $\sigma$  and  $\rho$  denote surface tension and mass density of the liquid and g the acceleration of gravity. This second assumption implies that the influence of gravity is negligible [23,34]. For a thin droplet with a small contact angle, the first assumption can be written as  $\epsilon = H/R \ll 1$ . These assumptions lead to a simplified form of the Navier-Stokes equation [35,16,17,36], where the radial velocity component *u* can explicitly be determined from the pressure p at the liquid–air interface.

The shape of the droplet h(r,t) is determined by conservation of mass, which incorporates changes in shape due to the flow inside the droplet and due to evaporation

$$\frac{\partial h}{\partial t} = \frac{1}{3\mu} \frac{1}{r} \frac{\partial}{\partial r} \left( r h^3 \frac{\partial p}{\partial r} \right) - J(r), \tag{1}$$

where  $\mu$  is the dynamic viscosity and J(r) indicates the evaporation velocity, which may depend on the radial coordinate. This equation holds for both pinned and unpinned contact lines. The pressure within the droplet is dominated by the effect of surface tension. At the liquid–air interface, the pressure difference between the droplet and the air is given by the Laplace pressure:

$$p = p_L = -\sigma \ \frac{1}{r} \ \frac{\partial}{\partial r} \left( \frac{r \ \frac{\partial h}{\partial r}}{\sqrt{1 + \left(\frac{\partial h}{\partial r}\right)^2}} \right). \tag{2}$$

The term in the denominator takes into account the exact radius of curvature of an axially symmetric drop and makes it possible to extend the range of validity of the approach to larger contact angles than possible when the lubrication approximation is made. Consequently, the equilibrium shape of the droplet is a spherical cap instead of a parabola, which is the equilibrium shape in the lubrication approximation.

For an unpinned contact line, the mass loss due to evaporation causes the contact line to move to the center of the droplet keeping a constant contact angle. However, at the contact line a singularity exists due to no-slip boundary condition at the liquid–substrate interface which is known as Huh and Scriven's paradox [18]. In Download English Version:

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