Numerical simulation of complex fluid drying in a Hele-Shaw cell

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Abstract. A 2D model is currently under development to describe the flow and concentration fields inside a Hele-Shaw cell with evaporation for a receding meniscus (dip-coating-like configuration). An original approach is proposed to address the difficult problem of the boundary conditions close to the contact line. The model is used to study the deposit thickness as a function of some process parameters.

1 Introduction

Dip-coating is a widely used industrial coating process, with complex coupling between hydrodynamics, mass transfer and evaporation, especially close to the contact line. Through various experimental and theoretical studies, it is now well established that different regimes appear depending on the Capillary number $Ca \equiv \mu V/\gamma$ ($\mu$ being the dynamic viscosity, $V$ the substrate velocity, and $\gamma$ the surface tension) [1–6]. At small Capillary number, viscous forces are strong enough to drag a liquid film whose thickness increases as $V^{2/3}$ (classical Landau-Levich regime). For even smaller Capillary numbers, another regime dominated by evaporation at the meniscus is encountered, characterized by a deposit thickness proportional to $V^{-1}$. Our objective is to build a hydrodynamic model of a dip-coating-like experiment (see reference [4]), in order to investigate the relation between the flow and the concentration field in the meniscus on one hand, and the deposit thickness on the other hand. In the present study which is a first step towards a more complete model of the process, we only take into account the flow driven by the substrate movement and the solvent evaporation. The free convection induced by buoyancy and/or Marangoni effect, which has been observed in the experiments, is temporarily disregarded. We focus on the difficult problem of the boundary conditions close to the contact line. An original approach based on lubrication approximation is presented, which avoids addressing stress and evaporative flux singularities, but still allows the prediction of the deposit thickness. This model may be viewed as the definition of the basic state for a future study of hydrodynamic instabilities in dip-coating processes.
2 Model

2.1 Geometry and assumptions

The model is based on experiments performed in a dip-coating-like set-up [4]. The device is made of two parallel glass plates separated by a gap $d$ which are vertically immersed in a reservoir filled with a solution of solute volume fraction $\phi_0$. Once the plates are immersed in the solution, there is a spontaneous capillary rise in the Hele-Shaw cell. The reservoir is then emptied at a constant pumping rate so that the position of the contact line decreases at velocity $V$. In our model, we consider the reverse equivalent configuration, i.e. the wall is moving upward with velocity $V$, while the meniscus is fixed. The mean evaporation velocity on the meniscus, $v_{ev}$, is controlled by a vertical air flow blown between the two glass plates, at a given temperature and humidity. A 2D domain is used to simulate the experimental setup (Fig. 1). The total height $H$ is large enough to get a fully developed flow at the bottom. The meniscus is assumed circular with radius $R$. Indeed, deformation induced by substrate motion or evaporation is located in the vicinity of the tip which is truncated in our model (cf. description below). For the complete wetting configuration considered in this study, $R = d/2 = 0.5mm$.

In the first step presented here, several simplifying assumptions have been made. Buoyancy, Marangoni effect and inertia are neglected. The solution density $\rho$ is a constant (same specific partial volume for the solvent and solute, so that the solvent (or the solute) mass and volume fractions are identical). The problem is isothermal.

To capture the basic characteristics of the local evaporation rate, i.e. a strong increase at the meniscus tip [6], the following expression is used: $j(m/s) = J_0/\sqrt{D_{tip}}$, where $D_{tip} = H - y$ is the distance to the tip of the contact line along the vertical axis. Note that this expression for the local evaporation rate is an approximation valid at the tip vicinity of the relation first suggested by Deegan et al. [7] for a sessile droplet. In this work, it is extended to the entire free surface, as a first step. $J_0(m^3/2s^{-1})$ is a constant deduced from the experimental value of $v_{ev}$ ($m/s$). $v_{ev}$ is obtained from preliminary experiments with pure water [4]. The dependence of the evaporation flux on the solute concentration is neglected.

Since the evaporation rate diverges at the tip, we define the truncated region shown in Fig. 1 by cutting off a small tip region whose height is $\alpha$ and width is $\delta$. The flow is assumed to be incompressible and the fluid to be Newtonian. Under these assumptions mass conservation and Stokes equations read in vector form:

$$\nabla \cdot \mathbf{v} = 0, \quad -\nabla P + \nabla \cdot (\mu \nabla \mathbf{v} + \mu \nabla^2 \mathbf{v}) = 0,$$

where $\mathbf{v} = u\mathbf{i} + v\mathbf{j}$ is the velocity field, $\mu$ is the viscosity (assumed constant in the following) and $P$ is the pressure. The mass balance for the solute reads:

$$\mathbf{v} \cdot \nabla \phi_p = D \nabla^2 \phi_p,$$

where $\phi_p$ is the volume fraction of solute and $D$ is the binary diffusion coefficient.

2.2 Boundary conditions

We assume no slip and impermeable boundary conditions at Boundary 1 and symmetry conditions at Boundary 3 (see Fig. 1). At $y = 0$ (Boundary 2) we consider a

$$v_{ev} = \frac{1}{R} \int_{\phi_{ev}}^{\phi_0} \frac{J_0}{\sqrt{H-y}} \frac{dy}{\sqrt{(H-y)(R-H+y)(R+H-y)}}$$

with $dy$ being an element of the free surface.