Contact line motion over heated substrates with spatially non-uniform wetting properties

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Abstract. We develop mathematical models of moving contact lines over flat heated solid surfaces with spatial variation of wetting properties under the conditions when evaporation is significant. The gas phase is assumed to be pure vapor and a lubrication-type framework is employed for describing viscous flow in the liquid. Substrate wetting properties are modeled through disjoining pressure, with the main focus on how the contact line motion changes near the regions of localized spatial variation of wetting properties.

1. Introduction

In heat transfer applications such as boiling or spray cooling, liquid-gas interfaces can come into contact with heated solid substrates [1-3]. Studies of solid surface non-uniformity and contact angle hysteresis [4] are important for many practical applications. The gas phase can be pure vapor or moist air, leading to different limiting mechanisms for local evaporation rates near contact lines. Several mathematical models of evaporation process from the liquid-gas interface in the contact line region have been developed over the past decades in order to describe coupling of evaporation and a number of other relevant physical phenomena such as capillarity, viscous liquid flow, London-van der Waals disjoining pressure, Marangoni stresses, diffusion and fluid flow in the gas phase, electrostatic interactions of interfaces, and vapor recoil. These studies address static and dynamic configurations for both triple lines, i.e. lines of contact of liquid, gas, and solid phases, and the so-called apparent contact lines, which are transition regions between macroscopic liquid-gas interfaces and ultra-thin films covering the solid substrate. The present study is focused on the latter case, illustrated in the sketch in Fig. 1; the gas phase is assumed to be pure vapor here and below. Local evaporation rate in this configuration has a maximum in the contact line region, while evaporation is completely suppressed in the ultra-thin film. Evaporative mass loss is compensated by the in-flow into the apparent contact line region.

The general framework for studies of the effect of evaporation on contact line motion for the case when the gas phase is pure vapor was provided by Ajaev et al. [5]. This paper deals with dynamics of vapor bubbles confined between two parallel walls. The interface shape is dominated by the capillary forces away from the walls, but the effects of viscous stresses, evaporation, and surface tension are all important near the walls. The apparent contact line model was used to define the moving boundary of macroscopically dry region of the wall. The main objective of the present study is to generalize the framework developed in Ajaev et al. [5] to include spatial variation of wetting properties of the...
substrate via appropriate modification of the disjoining pressure terms in the equations which describe the local interface shape near the contact line. The substrate temperature is assumed to be fixed, although the same framework can in principle be used to describe contact line motion over substrate with spatial variation of temperature and/or heat flux.

2. Model formulation

We consider a geometric configuration of a meniscus moving over a solid surface with spatially non-uniform properties. The meniscus radius of curvature $R$ away from the solid is constant (assuming that the appropriately defined Bond number is small enough for the effects of gravity to be negligible, which is typically a reasonable assumption for microsystems). Near the solid, the interface shape is affected by the viscous flow which in turn is coupled to the local evaporation rates from the interface. Evaporation here is assumed to be taking place in pure vapor environment. The solid substrate temperature is constant and higher than the vapor saturation temperature by the superheat value of $\Delta T$.

![Figure 1](image-url)

**Figure 1.** A sketch of geometric configuration of the apparent contact line region with solid substrates covered by ultra-thin adsorbed film.

The characteristic velocity $U$ is dictated by evaporation and thus can be estimated from the mass conservation condition at the interface where evaporation takes place. For evaporating liquid of density $\rho$ and thermal conductivity $k$ we can therefore write

$$U = \frac{k \Delta T}{\rho \ell R}$$

(1)

where $\ell$ is the latent heat of vaporization. For the geometric configuration considered, it is convenient to define nondimensional variables using the capillary number, which in turn is defined by the following equation,

$$C_a = \frac{\mu U}{\sigma}$$

(2)

Here $\mu$ is the dynamic viscosity of the evaporating liquid, $\sigma$ is the surface tension at the liquid-vapor interface. The capillary number is one of the key parameters in our formulation and provides a measure of relative importance of viscous effects and surface tension. Estimating the capillary number based on Eq. (2) for several liquids used in heat transfer applications shows that the numerical value of
this parameter is typically small. However, in the immediate vicinity of the contact line both viscous and surface tension effects can become important. To account for this, appropriate local Cartesian coordinates, shown in the sketch in Fig. 1, can be defined in terms of the capillary number by the following formulas,

\[ x = \frac{x^*}{RCa^{1/6}}, \quad y = \frac{y^*}{RCa^{1/3}} \]  

(3)

Here the asterisks denote dimensional variables. Note that for small capillary numbers, the horizontal length scale is much larger than the vertical one, so that using the lubrication-type approach is appropriate [6,7]. The details on the application of this approach to moving contact lines under the conditions when evaporation is taking place can be found in several recent works [5,8,9]. The key steps of the derivation in the present case are the same as described in e.g. Ketelaar and Ajaev [8] except that the disjoining pressure term is now a function of the local coordinate along the substrate. Also, for simplicity the disjoining pressure is assumed to only have one component, based on the London-van der Waals model of molecular interactions in the thin film. The final evolution equation for the local film thickness \( h \), scaled by the same characteristic value as the \( y \)-coordinate in Eq. (3) above, can then be written in the form

\[ h_t + J + \frac{1}{3} \left[ h^4 \left( h_{xx} + \frac{\alpha f(x)}{h^3} \right) \right] = 0 \]  

(4)

and the nondimensional evaporative flux \( J \) in this equation can be expressed in terms of the interface shape and various nondimensional parameters of the problem as follows,

\[ J = \frac{-\delta \left( h_{ss} + \frac{\alpha f(x)}{h^3} \right) + T_0}{K + h} \]  

(5)

Here the nondimensional parameter \( \alpha \) is the characteristic scaled Hamaker constant which measures the relative value of the London-van der Waals disjoining pressure; note that the dimensional values of the Hamaker constant have been measured for a wide variety of liquids on different substrates, as discussed e.g. in Israelachvili [10]. In the expression for the mass flux, we also introduced nondimensional parameters \( K, \delta \). The first one is the measure of the non-equilibrium effects due to evaporation at the interface, while the second defines the change in local equilibrium interfacial temperature due to changes in curvature and effects of disjoining pressure in the liquid. In all simulations reported below we use the following values: \( \alpha = 10^{-4}, K = 0.01, \delta = 10^{-4} \). The nondimensional quantity \( T_0 \) is the wall superheat scaled by the saturation temperature.

Numerical solution of the system defined by Eqs. (4)-(5) has been carried out using a finite-difference approach on the spatial interval \([-5, 5]\), with the boundary conditions of \( h(5) = 12 \) (fixed value to avoid multiple solutions in the limit of spatially uniform substrate) and \( h_{ss}(5) = 1 \) to account for constant curvature of the interface sufficiently far away from the wall (note that in the lubrication-type framework the interfacial curvature is well-approximated by the second derivative). At the left end-point of the computational domain, the conditions of zero first and third derivatives are imposed. Spatially non-uniform mesh was used to provide better resolution in the contact line region; the mesh size in that region is decreased by a factor of 8 compared to the rest of the simulation domain. The results shown below correspond to the total number of points in the coarse mesh equal to 1,000. Time stepping is performed using the subsroutines from the DVODE package with the initial condition
representing a parabola that satisfies boundary conditions at the right endpoint of the domain and the ultra-thin film patched together. The thickness of the ultra-thin film is determined from the condition of the evaporative flux $J$ in equation (5) (with $f(x)=1$) being equal to zero.

![Figure 2. Interfacial curvature profile for the wall superheat $T_0 = 0.01$ and spatially uniform substrate wetting properties](image)

3. Simulation results
Let us now discuss the numerical results. For all cases, the general outline of the procedure is as follows. We first find the steady-state solution corresponding to $T_0 = 0.01$ by running the code for sufficiently long time for the transients to decay. This situation corresponds to evaporation balancing the flow into the contact line region, meaning that the interface shape does not change with time. Curvature profiles for such steady state solutions typically have a well-defined maximum, as illustrated in Fig. 2. The scaled temperature is then instantaneously reduced by $\Delta T_0 = 0.006$, resulting in contact line motion to the left as suddenly weakened evaporation no longer compensates for the mass supply by the viscous flow. As the contact line moves, the interface profile also changes and these changes are recorded. The data on interface profiles at different moments in time is then used to track the motion of the contact line. Specifically, the position of the contact line is defined by the local maximum of curvature in the contact line region. For calculating this value, we first evaluate the curvature at every grid point and identify the point with the largest curvature value. Then, the local shape of the curve is approximated by a quadratic polynomial and the coordinate of the maximum of that polynomial graph is defined as the contact line location.

We first conduct simulations for the case when the substrate wetting properties are spatially uniform, so that $f(x) = 1$. The contact line location as a function of time for this case is shown by the dot-dashed line in Fig. 3, showing gradual slow-down as the new steady-state solution, corresponding to the smaller value of the wall superheat, is approached. The horizontal axis in Fig. 3 is the time measured from the moment of instantaneous change of the substrate temperature and scaled by the characteristic value of $R_0 Ca^{2/3}/U$; the maximum value of $t$ in the plot is chosen such that the system is close to the new steady-state solution; we verified that this is indeed the case by running the simulation up to a much higher value of $t = 100$. 
Figure 3. Evolution of the contact line position for spatially uniform substrate (dot-dashed line) and the case of an isolated defect (solid line) at $x_0 = 1$, as defined by Eq. (6).

Now consider the case when there is a localized region of variation of wetting properties, essentially a surface defect. This situation is modeled by a Gaussian profile so that the function $f(x)$ appearing in the equations above is defined by

$$f(x) = 1 - \frac{1}{2} \exp\left(-\frac{(x - x_0)^2}{(\Delta x)^2}\right)$$

with $x_0 = 1, \Delta x = 0.01$. The contact line position for this case is shown as a function of time by the solid line in Fig. 3. Clearly, as the defect is approached, the motion of the contact line slows down. However, after the contact line passed over the region of spatial non-uniformity, its speed increases. The two phases of motion, the slow-down and speed-up, do not entirely compensate each other as compared to the motion without the defect: the contact line ends up slightly further to the left.

The result for such modified configuration is shown in Fig. 4 and clearly corresponds to a significantly different behavior than seen in Fig. 3. The contact line slows down near $x = 1$ in a manner similar to the case of a single defect, but then instead of recovering and speeding up it slows down due to the interaction with the second localized region of the variation of wetting properties. The total contact line displacement at the point when the steady state is reached is in fact less than for uniform substrate.

Thus, depending on the nature of wetting properties variation, the contact line can be displaced either more or less that for the case of uniform Hamaker constant. Our observation from many simulations similar to the ones generating Figs. 3, 4 is that the outcome is very sensitive to the contact line speed in the region where local variation of the Hamaker constant is imposed. For the result shown in Fig. 4, the contact line speed is much slower near $x = x_1$ than near $x = x_0$, so the dynamics is different.
Figure 4. Evolution of the contact line position for spatially uniform substrate (dot-dashed line) and spatial variation of disjoining pressure modeled by two Gaussian profiles (solid line), one centered at $x_0 = 1$ and another one at $x_0 = 0.95$, as described by Eq. (7). Slow-down of the contact line is clearly seen.

4. Conclusions

We carried out a numerical investigation of contact line motion over a substrate with spatially non-uniform wetting properties. The fully unsteady lubrication-type model is developed which allows us to track evolution of the interface as a function of time in response to substrate temperature changes. The non-uniformity of substrate properties is modeled through the spatial variation of the Hamaker constant in the formula for disjoining pressure. The contact line speed at the time when the region of spatial non-uniformity is approached is identified as the key parameter determining the contact line dynamics. We started by considering a Gaussian profile of local spatial variation of the Hamaker constant. If the contact line is moving relatively fast, its slow-down due to local change in disjoining pressure is compensated by the subsequent speed-up in the region when the disjoining pressure is uniform again. However, if another region of spatial non-uniformity is encountered afterwards, the contact line can slow down significantly and its total displacement in response to temperature change will be less than for the case of spatially uniform substrate properties.

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