

Dynamic modelling of the deformed contact line under partial wetting conditions: quasi-static approach

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Abstract. We study numerically the motion of contact lines in the context of the "Wilhelmy plate" experiment: a vertical solid plate is withdrawn at constant velocity from a bath of liquid. We apply the contact line dissipation quasi-static model to the relaxation of the initially periodically deformed contact line. The obtained numerical data are compared to the experimental results [1] showing a good agreement.

The spreading of a liquid on a solid and the motion of contact lines are important in many industrial processes. That is why they are subject of numerous experimental and theoretical studies. It is important to achieve a certain degree of control over the spreading process and that involves also the motion of the contact line. This problem is especially challenging in the case of partial wetting regime where the singularity of the viscous dissipation appearing at the moving contact line need to be relieved with some model. A number of different approaches have been suggested in the literature. The testing of these approaches against the experimental data and determination of the range of validity of the approximations made is necessary. Our purpose is to test a contact line and wedge dissipation model [2,3] with respect to the recently obtained experimental data [1] on the receding motion of deformed contact lines in the "Wilhelmy plate" geometry. The contact line dissipation approach reduces the volume viscous dissipation that occurs in a vicinity of the moving contact line to the dissipation per unit length of the contact line localized *at* the contact line. Both viscous dissipation in the moving wedge described by de Gennes [4] and the dissipation due to the friction of the liquid molecules diffusing over the solid in the Blake-Haynes model [5], are proportional to the square of the local contact line velocity. We denote by $\xi/2$ the coefficient of proportionality. We would like to point out that this representation of the total dissipation is quite general (see [6,7], etc.). Starting from the variational principle of Hamilton and taking ξ into account, one arrives to the following (independent of the particular surface shape) equation, relating the local contact line velocity v to the local dynamic contact angle θ [8,9]:

$$v = \frac{\gamma}{\xi} (\cos \theta_{eq} - \cos \theta) \quad (1)$$

In the quasi-static approximation, the surface of the liquid is considered as if it were in equilibrium attained for the changing in time contact line position. The latter is determined with equation (1). Therefore, for an initially perturbed contact line, one needs to solve a genuine 3D problem to find the fluid surface (its shape and position) at each time moment.

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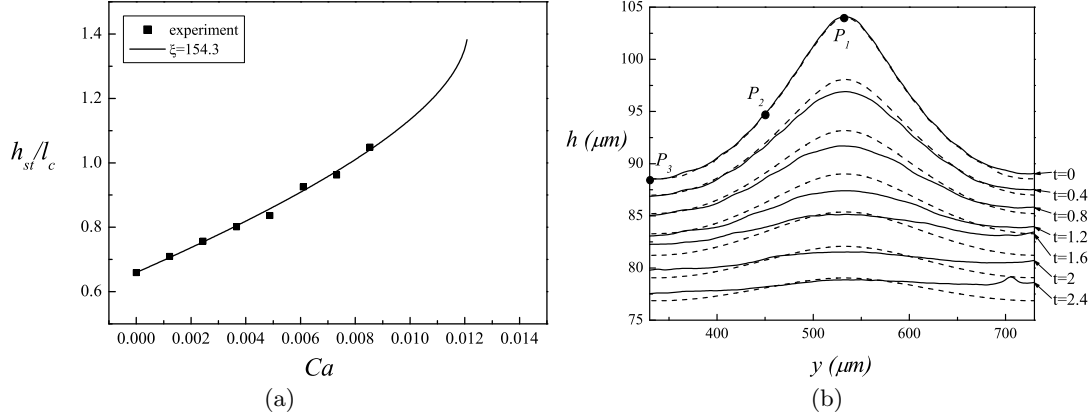


Fig. 1. (a) The stationary height of the contact line h_{st} (in the units of the capillary length l_c) as a function of the dimensionless plate velocity Ca . Squares: experiment [1]; line: eq. (2) with $\xi = 154.3$ Pa.s. (b) The contact line height $h(y, t)$ evolution at dimensionless velocity $Ca = 0.00476$ with time step $\Delta t = 0.4$ s. Only one period, of the initially periodically perturbed contact line with period $400 \mu m$ is shown. Dashed lines: numerical results; solid lines: experiment [1].

In this paper we consider the classical “Wilhelmy plate” experiment: a thin solid plate is withdrawn vertically at constant velocity u from a bath of liquid. One of the plate faces (we do not consider the other here) is described with the Cartesian coordinates (y, z) where the axis y is horizontal and the axis z is directed upwards. The liquid free surface forms with the moving plate a contact line L and dynamic contact angles $\theta(y)$ along the contact line. At the vertical bath wall opposite to the moving plate and parallel to it, the contact angle is assumed to be 90° . The distance between the plate and the wall is denoted d_x . We study the variable h which is the height of the contact line at the plate above the fluid surface at the opposite bath wall. Our study focuses on a specific system studied experimentally in [1] where h varies periodically along the contact line (i.e. $h = h(y, t)$) after its depinning from a horizontal row of periodical artificial heterogeneities on the plate. The period of the perturbation in [1] was $\lambda = 400 \mu m$. The goal of [1] and of the present work is the analysis of the contact line relaxation on a macroscopically homogeneous part of the plate with which the liquid surface forms a static receding contact angle $\theta_{eq} = 51.5^\circ$.

In order to determine how well this model reproduces the experimentally obtained results we need first to determine the value of the phenomenological dissipation coefficient ξ which is the only adjustable parameter of the model. ξ is determined from the experimental data on $h(y, t)$ measured as a function of the plate velocity u once the stationary value $h_{st} = h(t \rightarrow \infty)$ has been attained (see [10] for details). Obviously, h_{st} is independent of y and $v = u$ for this case since the contact line is immobile in the reference of the bath. h_{st} can be calculated from the static surface shape for which [7] $h_{st} = \sqrt{2(1 - \sin \theta)}$ where h_{st} is expressed in the units of the capillary length $l_c = \sqrt{\gamma/\rho g} = 1.46$ mm where the values of the surface tension $\gamma = 20.3$ mN/m, and density $\rho = 970$ kg/m³ correspond to that of the PDMS used in [1]; g is the gravity acceleration. The last equation implies $\cos \theta = h_{st} \sqrt{1 - h_{st}^2/4}$. Its substitution into (1) results in

$$Ca = \eta \left(\cos \theta_{eq} - h_{st} \sqrt{1 - h_{st}^2/4} \right) / \xi. \quad (2)$$

where $Ca = u\eta/\gamma$ is the capillary number and the shear viscosity [1] is $\eta = 4.95$ Pa.s. A fit of the experimental $h_{st}(Ca)$ data from Fig. 2a of ref. [1] with eq. (2) results in a value $\xi = 154.3$ Pa.s, see Fig. 1a.

We study next the relaxation dynamics of an initially perturbed contact line sliding down on a homogeneous plate pulled at constant velocity. We compare our results with the experimental results for the relaxation of an initially periodically perturbed contact line.

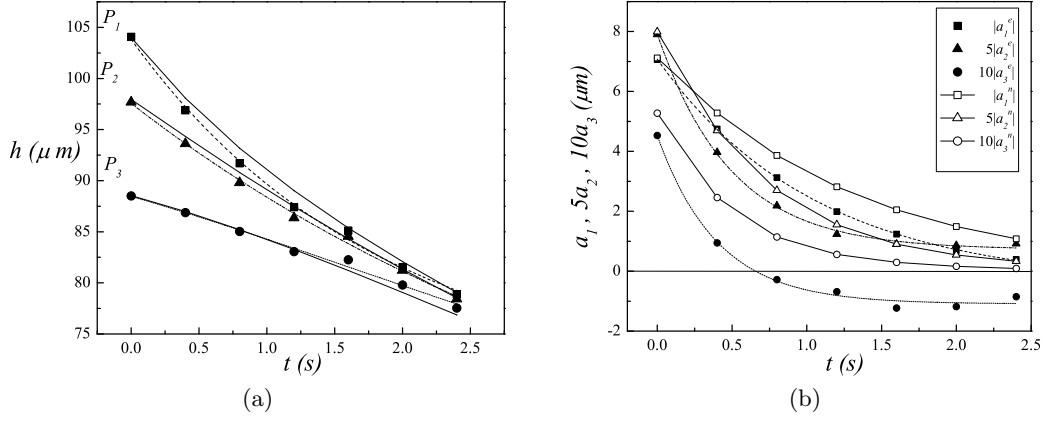


Fig. 2. (a) Time relaxation of the heights of the points P_1 , P_2 and P_3 from Fig. 1b. Solid lines: numerical results; characters: experimental results from [1] (P_1 : squares, P_2 : triangles, P_3 : circles); dotted lines: fits of the numerical results. (b) Time relaxation of the harmonic amplitudes a_1 , a_2 , and a_3 from eq. (3). The numerical results are shown by solid lines and by open characters. The experimental results are shown by the corresponding solid characters. $a_2(t)$ is multiplied by 5 and $a_3(t)$ by 10 in order to be of the same order of value as $a_1(t)$. The dashed lines are the fits of the experimental data.

The numerical algorithm we use is similar to that of [8]. The liquid surface is approximated by a set of triangles with vertex points $R[x_i, y_j, z(x_i, y_j)]$; $i = 1, \dots, N_i$; $j = 1, \dots, N_j$, where $N_j = 51$. This choice is imposed by the necessity to resolve the contact line curvature. We obtained solutions for $N_i = 400$ ($d_x = 7.3l_c$), $N_i = 500$ ($d_x = 12.3l_c$), $N_i = 600$ ($d_x = 17.3l_c$) to check the independence of the relaxation time of the contact line of d_x . The corresponding values differ less than 5%.

The contact line evolution is shown in Fig. 1b for one specific velocity of the plate $Ca = 0.00476$. For the sake of easier comparison we have also reproduced the experimental profiles from Fig. 5b of [1] for $y \in [330, 730] \mu\text{m}$.

To start the numerical simulation we need to define an initial contact line position. The experimental contact line at time $t = 0$ (see Fig. 1b) is not exactly periodical: the point at $y = 730 \mu\text{m}$ is misplaced to about $1.23 \mu\text{m}$ with respect to the point at $y = 330 \mu\text{m}$. However we need an initially periodic contact line for the simulation. We generate an initial contact line which in the interval $y \in [330, 600] \mu\text{m}$ coincides with the experimental contact line and then is smoothly continued in the interval $y \in [600, 730] \mu\text{m}$ so that its height at the end point is equal to height at the initial point.

In Fig. 2a the time relaxation of the heights of the three points P_1 , P_2 and P_3 (see Fig. 1b) of the contact line is shown. P_1 (with $y = y_1 = 530 \mu\text{m}$) is the maximum, P_2 ($y_2 = 474 \mu\text{m}$) is an intermediate point, and P_3 ($y_3 = 330 \mu\text{m}$) is the minimum of $h(y)$. We compare their relaxation by using the fitting functions to the numerical and the experimental data. The functions $h(y_{1,2}, t)$ are very well fitted by the exponential relaxation in the time interval $t \in [0, 2.4] \text{ s}$ for both the numerical and experimental sets of data. The relaxation times for P_1 are 2.83 s from the experimental and 2.88 s from the numerical results. For the point P_2 one gets 3.44 s and 3.46 s respectively. The time relaxation of the point P_3 is different. Its inverse height, i.e., $[B - h(y_3, t)]^{-1}$ is well fitted by the exponential decay function with $B = 90 \mu\text{m}$ and the relaxation times 0.46 s for the experimental and 0.48 s for the numerical data. One sees, that the numerical and experimental relaxation times of the points P_1 , P_2 and P_3 differ by less than 2-4%. This clearly shows that the contact line dissipation model describes quite well the time evolution of the relaxing deformed contact line.

As suggested in [1], we fit now the profiles of the contact lines with a three mode Fourier decomposition

$$h(y, t) = a_0(t) + a_1(t) \cos(q_0 y + y_0) + a_2(t) \cos(2q_0 y + y_0) + a_3(t) \cos(3q_0 y + y_0). \quad (3)$$

Note that the experimental results are obtained only for the time interval $t \in [0, 2.4]$ s while in the numerical simulations we continue the simulation to much later times.

The results for the time evolution of $a_1(t)$, $a_2(t)$, $a_3(t)$ are displayed in Fig. 2b. The upper index is n for the numerical and e for the experimental values.

The numerical data are fitted well enough with the exponential decay functions (with zero free term) with the relaxation times 1.28, 0.73, 0.52 s for $a_1^n(t)$, $a_2^n(t)$, $a_3^n(t)$ respectively. The times do not follow the proportionality pattern $1 : 1/2 : 1/3$ that would be expected [11] within the linear approach which holds asymptotically for small liquid surface slope that can be estimated by $\partial h / \partial y$. This deviation can be explained by the significant value of $\partial h / \partial y$ which defines the contribution of nonlinearity to the surface curvature that governs the surface relaxation. At $t = 0$ $\partial h / \partial y$ attains 0.12. On the late stages of relaxation, it becomes much smaller (see Fig. 2b) and, according to this reasoning, the relaxation should obey better the linear theory. Indeed, for $t \in [3.6, 5.6]$ s, the exponential fitting results in the relaxation times 1.21, 0.64, 0.403 s which satisfy the proportionality pattern $1 : 1/2 : 1/3$ much better than the early stage results.

The quality of the exponential fit of the experimental data decreases with the number of the harmonics because the higher harmonics are influenced stronger by the non-smoothness of the contact line profiles due to the small scale surface heterogeneity. We obtain 1.07, 0.49, 0.4 s for the relaxation times of the functions $a_1^e(t)$, $a_2^e(t)$, $a_3^e(t)$ respectively. These relaxation times are close to the numerical relaxation times obtained on the late stages. When one uses a Fourier decomposition of the contact line only on the interval $[330, 530]$ μm (half period) to eliminate the impact of the asymmetry of the experimental contact line, the corresponding times approach the numerical early stage results. They do not follow the proportionality pattern $1 : 1/2 : 1/3$ either.

In conclusion, the numerical data obtained with the contact line dissipation model compare very well with the experimental results. A single adjustable parameter, the dissipation coefficient ξ can be obtained from the data on relaxation of the straight contact line with good accuracy and is sufficient to explain the motion of the deformed contact line. A good (within 2-4%) agreement of the contact line profiles and relaxation times obtained from the experimental and numerical data sets shows that the quasi-static approach can be used for the description of the contact line dynamics in the partial wetting regime.

Note, that the contact line dissipation approach is tested here in the most unfavorable for the model situation. Because of the high viscosity of the silicon oil used in [1], the geometrical region where the dissipation is important extends to a relatively large volume of the fluid. Our approach should work even better for more common low viscosity fluids like water or alcohol where the dissipation is stronger localized at the contact line.

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