The dynamics of the triple gas-liquid-solid contact line is analysed for the case where the gas is the saturated vapour corresponding to the liquid, like in the vapour bubble in boiling. It is shown that even small superheating (with respect to the saturation temperature) causes evaporation of the adsorption liquid film and the true triple contact is established. It is shown that the hydrodynamic contact line singularity cannot be relaxed with the Navier slip condition under such circumstances. Augmented with the second derivative slip condition is proposed to be applied. For the partial wetting conditions, a non-stationary contact line problem where the contact line motion is caused by evaporation or condensation is treated in the lubrication approximation in the vicinity of the contact line. High heat fluxes in this region require the transient heat conduction inside the heater to be accounted for. Two 2D problems, those of drop retraction with no phase change and of drop evaporation are solved and analysed as illustrations of the proposed approach.
1. Introduction

The modeling of bubble growth remains to be poorly understood in spite of its importance for estimation of the overall heat transfer during the nucleate boiling. It is widely recognised that a large part of the boiling heat transfer is due to the evaporation at the foot of the bubble, in the region often called “microregion”. Therefore a poor knowledge of the microregion processes can lead to a large uncertainty of the overall heat transfer estimations.

One of the most important advances in the understanding of this problem and of the boiling in general has been made by Cooper & Lloyd (1969) when they suggested the existence of a thin liquid layer (“microlayer”) that separates the bubble from the heater. They have based their conclusion on the hemisphericity of the bubbles. As a matter of fact, the bubbles become hemispherical under the action of the inertial hydrodynamic forces which are important when the bubbles grow fast enough, that is at low system pressures.† The present understanding of the study of the microlayer evaporation is based on the approach developed originally by Wayner et al. (1976) for the evaporation of the continuous liquid meniscus. Among numerous applications of these ideas in boiling and evaporation in general one can cite the works of Stephan & Hammer (1985), Son & Dhir (1999), Morris (2000), Ajaev et al. (2002). In these theoretical and numerical studies it was assumed that the thinnest part of the microlayer (“adsorption film”) does not evaporate due to the van der Waals attraction forces that exist between the molecules of the solid heater and the fluid.

While the theoretical and numerical studies deal with the continuous microlayer, ex-
† At high pressures (i.e. comparable with the critical pressure for the given fluid), the bubble shape is rather spherical than hemispherical. Cooper and Lloyd were cautious about applicability of their idea to this case.
Experimentalists speak about “dry spots” under the bubbles that are most easily observed (van Ouwerkerk 1972; Torikai et al. 1991; Theophanous et al. 2002; Hegseth et al. 2005; Nikolayev et al. 2006) when the heat flux transferred from the heater to the fluid is comparable to the critical heat flux (CHF) at which the heater dries out and the transition to the film boiling takes place. This phenomenon is called “boiling crisis” or “departure from nucleate boiling”. To predict the CHF, the understanding of the drying dynamics is essential (Nikolayev & Beysens 1999; Nikolayev et al. 2001). It is likely that dry spots exist at much smaller fluxes however they are smaller and thus more difficult to observe.

The drying implies the direct contact of the vapour with the solid and the existence of the triple vapour-liquid-solid contact line (CL). The determination of the CL position becomes a key to the dryout simulation and requires the clear understanding of the heat transfer near the CL, which is the subject of this article. In the next section we discuss the conditions under which the CL concept is relevant.

Besides the description of drying, the CL issue is important for the understanding of the bubble departure from the heater, another key feature of boiling. The surface tension is the only force that provides the adhesion of the bubble at the last, thermally controlled stage of the bubble growth (Son & Dhir 1999). This force exists only when the CL exists and is proportional to its length. The CL position is thus needed to be known to assess the bubble departure size.

High heat fluxes that occur in the microregion show the importance of the accounting for the thermal conduction in the heater that influences strongly the evaporation rate at the bubble interface (Nikolayev et al. 2001). It has not been taken into account in the previous studies of the microregion and will be discussed in the present work.

The hydrodynamic stresses are well known to be infinite at the moving CL when the classical no-slip boundary condition (zero tangential velocity at the solid wall) is applied.
This non-physical singularity need to be relaxed. The replacement of the no-slip condition by the Navier slip condition presents a singularity relaxation solution that is used by most researchers working in this field. In sec. 4.1 we show that this solution in inappropriate when heat transfer is taken into account. We propose a new slip boundary condition that allows the CL singularity to be relaxed self-consistently.

Two coupled parts of the CL problem can be distinguished: the heat transfer problem which is dealt with in the section 3 and the determination of the shape of the liquid-vapour interface near the CL discussed in the section 4. However one needs to analyse first the conditions at which the liquid film at the heater dries out and the CL actually appears.

2. Does the adsorption liquid film exist at the heater?

Numerous experimental studies have been carried out to detect the dry spots on the hot enough heater. In the experiments (van Ouwerkerk 1972; Torikai et al. 1991) with a transparent heater the total internal reflection at the heater-fluid interface was used to detect the dry spots. This shows that even if the liquid film existed, its thickness was smaller than the about one tenth of the light wavelength ($\sim 50$ nm). In the experimental study of evaporation at extremely high (nearly critical) pressures (Hegseth et al. 2005), the motion of the CL separating the wetted and dry areas have been studied optically, with about the same precision. In order to check if the thinner film exist, only molecular dynamics simulations data is available. Most simulation studies (Maruyama & Kimura 2000; Consolini et al. 2003) show only separate molecules adhering to the solid so that the continuous liquid layer is nonexistent. The liquid layer was rather thick in the simulations of Freund (2005) but only the case of almost insignificant superheating have been studied.

In the absence of the other data, let us analyse this problem theoretically. The studies
Dynamics of the triple contact line on the non-isothermal heater of thin films evaporation analogous to those by Wayner belong to the class of the “mean field” theories. This term comes from the statistical physics and means that the thermal fluctuations are neglected. It is well known that the fluctuations can be neglected for large systems. In the present context, “large” means that the number of the molecular layers in the film is large. Let us estimate the film thickness for which the thermal fluctuations need to be taken into account.

The van der Waals energy of a fluid molecule situated at a distance \(d\) from the half-space filled with the material \(j\) can be calculated as (Israelachvili 1992)

\[
W_j(d) = -B F_j n_j \pi \frac{\pi}{6d^3}, \tag{2.1}
\]

where \(n_j\) means the number of molecules per unit volume, \(S\) or \(L\) should be used instead of \(j\) depending on if the half-space is filled by solid (i.e. heater) or liquid respectively, \(B\) is the constant of \(r^{-6}\) attraction between respective molecules. Note that the expression for the disjoining pressure \(p_d = A/d^3\) can be calculated from (2.1).

It is evident that the van der Waals forces cannot hold the fluid molecules at any superheating: at some temperature the kinetic energy of the molecules (usually neglected in the previous analyses of the adsorption films) will become so high that they will leave the heater. In order to find at which superheating the adsorbed liquid film will disappear, one needs to compare the cohesion and thermal (kinetic) energies for a molecule sitting at the vapour-liquid interface. Compare two configurations (Fig. 1). The first is the plane vapour-liquid interface at saturation temperature \(T_{sat}\) (Fig. 1a). In the second configuration, a part of the lower half-plane situated at the distance \(d\) from the interface is replaced by a solid heater so that a liquid film is formed (Fig. 1b). The change of cohesion energy of an interface probe molecule between two these configurations is

\[
\Delta W(d) = W_L(d) - W_S(d) = (B_{FS}n_S - B_{FF}n_L) \frac{\pi}{6d^3}, \tag{2.2}
\]
The excess kinetic energy gained by this probe molecule due to the larger (for the second configuration) interface temperature $T^i$ is $k_B(T^i - T_{sat})$, where $k_B$ is the Boltzmann constant. By solving the equation $\Delta W(d) = k_B(T^i - T_{sat})$ for $d$, one obtains the critical thickness $d_c$. The molecules situated at larger distances are not kept by the van der Waals forces in the film and are evaporated.

To obtain the upper bound for $d_c$, we assume the extreme case $B_{FS}n_S \gg B_{FF}n_L$ that strongly favours the wetting film formation. By using the order of value estimations (Israelachvili 1992) $n_S \sim 10^{29} \text{ m}^{-3}$ and $B_{FS} \sim 10^{-77} \text{ J} \cdot \text{m}^6$, one obtains $d_c = 3 \text{ nm}$ for the superheating $T^i - T_{sat} = 1^\circ \text{C}$. Since for such thin films the temperatures of the interface and of the heater almost coincide and the local superheating attains often much larger values, $d_c$ value in reality is even smaller. Such films adhere rather than flow (Freund 2005). As far as the fluid flow is concerned, their existence can thus be neglected. The conclusion is that even small superheating causes complete evaporation of the liquid film and formation of the CL. Therefore the classical theory of meniscus evaporation from which the CL is absent (the “interline” was defined in these models as a contact between the vapour, bulk liquid and the film) needs to be revisited. The term “microregion” will be used below to denote the vicinity of the CL.
When the CL is present, one cannot use the diverging at $d \to 0$ expression for $p_d$. It must be corrected for the short range intermolecular interactions to describe self-consistently the partial wetting case (Brochard-Wyart et al. 1991). However the disjoining pressure ceases to be an important factor for the wedge geometry. Indeed, the area where $p_d$ is significant ($h < 100$ nm) is very small. Following previous works on the treatment of heat transfer in the case where the CL is present (Anderson & Davis 1995), we thus omit $p_d$ from further consideration.

3. Heat transfer in the microregion

In the description of the microregion, the curvature of the vapour-liquid interface in the direction parallel to the CL can be neglected with respect to the curvature $K$ in the perpendicular direction. The interface can thus be described by its 2D contour (Fig. 2). We shall assume that the contact angle $\theta \neq 0$ is small (which is generally the case for most heaters) so that the slope of the interface is small. The interface can then be described by its height $y = h(x)$ and the small slope assumption means $|\partial h/\partial x| \ll 1$. All the variables can then be described as functions of $x$. 

Figure 2. Geometry of the general problem. The chosen direction of the normal to the interface is shown.
3.1. Problem statement in a general case

The most na"ive approach to the contact line heat transfer would be assuming both the liquid-vapour and liquid-heater interfaces isothermal. The background argument is that the temperature of the vapour-liquid interface $T_i$ is generally very homogeneous (Marek & Straub 2001; Barthes et al. 2007) ($T_i = T_{sat}$) in the absence of impurities in both liquid and vapour phases (which is the case considered here). On the other hand, the surface of the metal heater is often assumed isothermal due to its high thermal conductivity. To vaporise the liquid, the heater surface temperature $T_S$ needs to be higher than $T_{sat}$. Since the CL belongs to both interfaces, its temperature is ambiguous, which is well known to generate the non-integrable divergence of the heat flux at the vapour liquid interface (assumed to be positive at evaporation) $q^i_L(x) \sim 1/x$, which means that the integral heat balance cannot be satisfied at all. To avoid this difficulty, the temperature needs to be allowed to vary along at least one of the interfaces.

$T_i$ can only vary due to kinetic effects that are taken into account by introduction of the interface resistance $R^i$ (Stephan & Hammer 1985),

$$T^i = T_{sat}^p + R^i q^i_L,$$

(3.1)

where

$$R^i = \frac{T_{sat} \sqrt{2\pi R_g T_{sat}/M(\rho_L - \rho_V)}}{H^2 \rho_L \rho_V};$$

$M$ is the molar weight, $R_g$ is the universal gas constant, $H$ is the latent heat and $\rho_L$ ($\rho_V$) is the liquid (vapour) density. Rather than the saturation temperature for the given system pressure $T_{sat}$, (3.1) involves the saturation temperature

$$T_{sat}^p = T_{sat} \left(1 + \frac{\Delta p}{H \rho_L}\right),$$

(3.2)

that depends (Wayner et al. 1976; Stephan & Hammer 1985) on the pressure jump $\Delta p = p_V - p_L$ across the interface. $\Delta p$ includes contributions of all forces that act on the system.
If other forces like gravity, van der Waals forces, electric field, etc. were considered, they would need to be accounted for in (3.2). It is obvious from the following *ad absurdum* argument valid for the interface at equilibrium. Indeed, if some forces were omitted from (3.2) but present in the force balance, (3.1) would result in the $\Delta p$ and $T^i$ variations along the interface. However according to the equilibrium condition, both temperature and pressure need to be homogeneous. The $T^i$ variation can appear only when the evaporation creates the viscous pressure drop due to the fluid flow as shown below in (4.10).

In principle, the boundary condition (3.1) is sufficient to relax the CL singularity and simulate the bubble growth on the isothermal heater. However the heat flux $q^i_L$ (and thus the bubble growth rate) would be then overestimated because in reality the heater temperature in the vicinity of the CL varies strongly, see sec. 5.5. In a more realistic modeling, the heat conduction in the heater needs to be taken into account so that both vapour-liquid and liquid-solid interface temperatures allowed to vary.

Morris (2000); Ajaev et al. (2002) assumed the stationary temperature distribution inside the heater. However, it is never stationary because the characteristic heat diffusion length $\sqrt{\alpha_S t}$ (where $t$ is the bubble growth time and $\alpha_S$ is the heater material temperature diffusivity) is usually comparable to a characteristic system size. E.g. for the bubble growth problem this size is the bubble radius the dynamics of which is controlled by the heat supply from the heater. Another reason is that the temperature distribution in the heater cannot accommodate instantaneously the changes in geometry caused by the CL motion. Below we study a *transient* heat conduction problem in a semi-infinite heater with an arbitrary distribution of the heat flux $q_S(x,t)$ at the heater surface. $q_S$ will be determined later on by matching with the liquid domain solution.

The energy is supplied to the heater via a homogeneous volume heating (by the electric current). In the framework of the present approach any time dependence of the volume
heating power can be treated. The heating power per unit volume is chosen in the form \( C/\sqrt{t} \) to model a heating impulsion at \( t = 0 \); \( C \) is an arbitrary constant. Although by other reasons, the same form has been chosen by Nikolayev et al. (2001). As in that article, the reference heat flux can be defined via \( C \) as

\[
q_{ref} = C \sqrt{\pi} \alpha_S k_L / (k_S \sqrt{\alpha_L} + k_L \sqrt{\alpha_S}),
\]

where \( k \) means the heat conductivity of the liquid \( (k_L) \) or solid \( (k_S) \).

The homogeneous initial temperature \( T_S(t = 0) = T_0 \) is chosen as the initial condition.

The resulting temperature of the heater surface obtained with the Green function method (Carslaw & Jaeger 1959) is then

\[
T_S(x, t) = T_0 + \frac{2 \alpha_S C \sqrt{t}}{k_S} - \frac{1}{2 \pi k_S} \int_0^t \int_{-\infty}^{\infty} q_S(x', \tau) \exp \left[ -\frac{(x - x')^2}{4 \alpha_S (t - \tau)} \right] dx'.
\]

The \( T_0 \) value

\[
T_0 = T_{sat} \left( 1 + \frac{\Delta p_0}{H \rho_L} \right)
\]

is chosen to be equal to the saturation temperature corrected for the initial pressure jump \( \Delta p_0 \) appearing due to the initial interface curvature. The following assumptions are made to solve the conjugated problem in the whole domain.

- The temperature distribution across the liquid film is assumed to be stationary.

This approximation is valid when the film thickness is smaller than the thermal diffusion length \( \sqrt{\alpha_L t} \). The heat flux is then constant across the liquid and

\[
q_S(x) = q_{L}^i(x) = k_L \frac{T_S(x) - T^i(x)}{h(x)}.
\]

- The vapour is assumed to be non conductive. The heat flux to the vapour domain is then neglected at the part of the heater surface in contact with vapour. The infinite coordinate integration limits in (3.4) needs to be replaced by the liquid-solid contact area \( \Omega_{LS} = \Omega_{LS}(t) \) because \( q_S \) vanishes at the rest of the heating surface.
By using (3.1, 3.2, 3.6), one obtains the expression

\[ T_S(x) = T_{sat} \left( 1 + \frac{\Delta p(x)}{H \rho_L} \right) + q_S(x) \left( R^i + \frac{h(x)}{k_L} \right), \] (3.7)

where all the variables are taken at the same time moment. Equalising with (3.4) leads to the following integral equation for \( q_S(x, t) \):

\[ q_S(x, t) \left[ R^i + \frac{h(x, t)}{k_L} \right] + q_{sat} \left[ \Delta p(x, t) - \Delta p_0 \right] = \frac{2 \alpha_S}{k_S} C \sqrt{t} \]

\[ \frac{1}{2 \pi k_S} \int_0^t \int_{\Omega_{LS}(\tau)} q_S(x', \tau) \exp \left[ -\frac{(x - x')^2}{4 \alpha_S (t - \tau)} \right] dx', \] (3.8)

which needs to be solved only for \( x \in \Omega_{LS}(t) \).

An important consequence of this quite general heat transfer model consists in the following: the pressure jump \( \Delta p \) should be finite everywhere, otherwise the temperature \( (3.7) \) will be infinite, which is non-physical.

4. Interface shape determination in the microregion

4.1. Relaxing the hydrodynamic CL singularity

Generally speaking, the interface shape is determined from the solution of the equations of hydrodynamics in the liquid and vapour domains with the appropriate boundary conditions. The viscosity and the inertia of the vapour can be neglected with respect to those of the liquid. The equations of hydrodynamics in the vapour then lead to the homogeneous vapour pressure \( p_V \). Analogously to the thin films treatment (Wayner et al. 1976; Stephan & Hammer 1985; Hocking 1995; Anderson & Davis 1995), the hydrodynamics equations in the liquid in the vicinity of the CL can be solved using the lubrication approximation. The jump of the normal stress reduces to the pressure jump \( \Delta p \) at the interface because the normal viscous stress is negligible in the lubrication approximation. For solving the lubrication equations, the boundary condition for the tangential velocity \( v_x \) at the solid surface is necessary to be defined among others. This condition turns out
to be extremely important when the CL is allowed to move. It is well known that the conventional no-slip condition

\[ v_x = 0 \] (4.1)

leads to a non-integrable divergence of the stress at the CL so that the force balance (see (4.11) below) cannot be satisfied. The simplest (and for this reason used by many researchers) method of relaxing this singularity consists in using instead of (4.1) the Navier slip condition

\[ v_x = l_s \frac{\partial v_x}{\partial y} \] (4.2)

that involves the slip length \( l_s \), which is reviewed in detail by Lauga et al. (2007). A conventional approach that makes use of the lubrication approximation (see Appendix A) shows that the corresponding to (4.2) pressure jump is defined by the equation

\[
\frac{\partial}{\partial x} \left[ h^2 \left( \frac{h}{3} + l_s \right) \frac{\partial \Delta p}{\partial x} \right] = \mu \left( v^i - \frac{q^i_L}{\rho L H} \right),
\] (4.3)

where \( v^i = v^i(x) \) is the interface velocity. The case \( q^i_L = 0 \) of (4.3) has been derived by Snoeijer et al. (2007) to describe the contact line motion with no phase change.

The case \( q^i_L = 0, l_s = 0 \) is conventional for the description of the motion of the continuous thin films. Another limit \( v^i = 0, l_s = 0 \) has been used by Wayner et al. (1976); Stephan & Hammer (1985); Hocking (1995); Anderson & Davis (1995). A similar to (4.3) approach (derived from more general Stokes equation) has been discussed by Mathieu et al. (2002) who also aimed to describe the contact line evaporation. They however considered \( l_s = 0 \); the CL singularity has not been solved. It should be noted that \( q^i_L \) and \( v^i \) are not independent in the case considered here: the interface moves due to evaporation. Similarly to the approach of Ajaev et al. (2002), both \( q^i_L \) and \( v^i \) are allowed to vary along the interface.

Before starting the numerical calculation, an asymptotic approach needs to be per-
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formed at $x \rightarrow x_{CL}$ to determine whether divergencies are encountered. Since $q_i^L(x) = q_S(x)$ is required to be bounded (by the same reasons as $\Delta p$), the r. h. s. of (5.6) needs to be considered constant in this limit because of the finite value of the contact line velocity.

Close to the CL,

$$h \sim \theta(x - x_{CL})$$

(4.4)

and the first integration of (4.3) results in

$$h^2 \left( \frac{h}{3} + l_s \right) \frac{\partial \Delta p}{\partial x} \sim (x - x_{CL}).$$

(4.5)

The subtraction of $x_{CL}$ (which is the integration constant) in the r. h. s. is necessary to match the zero value of the l. h. s. at $x = x_{CL}$. By using (4.4) in (4.5), one arrives to the asymptotic expression

$$\frac{\partial \Delta p}{\partial x} \sim \frac{1}{x - x_{CL}},$$

(4.6)

which results in $\Delta p \sim \log |x - x_{CL}|$. Being integrable, this divergence does not pose any conceptual problems for the conventional description of the moving CL with no mass transfer (Hocking 1995; Snoeijer et al. 2007). For the case of the phase transition at the interface, the pressure is however required to be finite at the CL because it determines the local interface temperature, see (3.1-3.2). The Navier slip condition (4.2) is thus unsatisfactory.

The method of relaxing of the CL singularity proposed by Shikhmurzaev (1997) does provide a finite pressure at the CL. However we shall not use this method here because of its high complexity: it involves additional physical assumptions and requires several more equations to be solved in addition to the conventional hydrodynamics. We propose instead a modification of the slip boundary condition. The physical significance of the

† This divergence however does lead to poor convergence of the numerical solution of transient problems, see sec. 5.4.
condition (4.2) is transparent. It means simply a linear mobility relation between the force exercised on the liquid (i.e. the hydrodynamic stress) and the velocity. The first choice would be to assume a nonlinear law (the force proportional to some power of the velocity). However, it can be shown (see Appendix B) that such a boundary condition leads to the logarithmic divergence too. We propose to use instead of (4.2) the “second derivative” boundary condition

\[ v_x = l_s \frac{\partial v_x}{\partial y} - \beta l_s^2 \frac{\partial^2 v_x}{\partial y^2}, \]  

(4.7)

where \( \beta \) is a constant. The second term involves the normal derivative of the tangential viscous stress while the first involves the viscous stress itself. This condition is used (Maurer et al. 2003; Hadjiconstantinou 2003; Lockerby et al. 2004) to describe high velocity gas flows. Although the velocities are far from being high in the present case, the second derivative term is needed to be accounted for because the stresses are large near the CL. The stress normal derivative is negative because the shear stress is a decreasing function of the distance from the wall.

A condition that involves the second velocity derivative is not a natural boundary condition for the Navier-Stokes equations. Strictly speaking, the higher order (and for this reason much more complicated) Burnett equations ought to be solved instead. However there are no technical interdictions to use the condition (4.7) with the Navier-Stokes equations and it is often done in practice (Maurer et al. 2003). This way will be followed here too. According to Hadjiconstantinou (2003), the value \( \beta = 0.5 \) fits well the results of numerical simulations; it will be used hereafter.

The pressure jump corresponding to the second derivative slip condition (4.7) is defined by the expression (see Appendix A for its derivation)

\[ \frac{\partial}{\partial x} \left[ h \left( \frac{k^2}{3} + hl_s + \beta l_s^2 \right) \frac{\partial \Delta p}{\partial x} \right] = \mu \left( v^i - \frac{q_i}{\rho_L H} \right). \]  

(4.8)
When performing the asymptotic analysis of this equation, one notices that the term $\frac{\beta l^2_s}{s}$ in the parentheses of the l.h.s. is prevailing and causes the finiteness of $\frac{\partial \Delta p}{\partial x}$ when $x \to x_{CL}$.

$$
\frac{\partial \Delta p}{\partial x} \bigg|_{x \to x_{CL}} = \frac{\mu}{\beta \theta l^2_s} \left[ \frac{v^i(x_{CL}) - \frac{q^i_L(x_{CL})}{\rho_L H}}{\rho_L H} \right].
$$

The pressure jump $\Delta p(x_{CL})$ is thus finite and (4.8) can be used to describe evaporation in the microregion. For the numerical treatment of (4.8), it is convenient to enforce the condition (4.9) by integrating (4.8) once, which results in

$$
h \left( h^2 \frac{2}{3} + hl_s + \beta l^2_s \right) \frac{\partial \Delta p}{\partial x} = \mu \int_{x_{CL}}^{x} \left[ \frac{v^i(x') - \frac{q^i_L(x')}{\rho_L H}}{\rho_L H} \right] dx'.
$$

4.2. Interface shape equation

The pressure jump $\Delta p$ across the interface can be written as

$$
\Delta p = K \sigma - p_r,
$$

where $K$ is the interface curvature, $\sigma$ is the surface tension and $p_r = \eta^2(\rho_v^{-1} - \rho_L^{-1})$ is the differential vapour recoil pressure which needs to be taken into account when the heater drying is considered; $\eta$ is the local mass exchange rate, see (A.10).

In 2D case Eq. (4.11) reads

$$
\sigma \frac{\partial^2 h}{\partial x^2} (1 + u^2)^{-3/2} = \Delta p + p_r,
$$

where $u = \partial h/\partial x$. The boundary conditions at $x = x_{CL}$ for (4.12) are given by two expressions

$$
h = 0,
$$

$$
u = \tan \theta.
$$

The contact angle $\theta$ depends only on the materials of the tree phases at contact as given by the classical Young formula. Since $\theta$ and the interface slope in the microregion are
usually small, Eq. 4.12-4.14, reduce to

\[ \sigma \frac{\partial^2 h}{\partial x^2} = \Delta p + p_r, \quad (4.15) \]

\[ h = 0 \text{ and } u = \theta \text{ at } x = x_{CL}. \quad (4.16) \]

Note that the interface shape changes with time because of the time variation of the pressure terms. The set of equations (4.10) (where \( q_S \) is used for \( q_L \)) and (3.8, 4.15, C3) allows the heat transfer in the microregion to be determined. One more remark concerns the CL time evolution \( x_{CL} = x_{CL}(t) \) that obeys the equation

\[ \frac{dx_{CL}}{dt} = \frac{v'(x_{CL})}{\theta}. \quad (4.17) \]

It follows from (4.16, C1, C3) since the condition \( \frac{dh}{dt} = 0 \) holds at the CL.

One more equation is necessary for the problem closure. For example in the bubble growth problem (Kern & Stephan 2003), the matching of the solutions in the microregion (where the thin film approximation is applicable) and the rest of the bubble interface (macroregion) is required.

5. Hydrodynamics and heat transfer during the evaporation of a shallow droplet

The drop evaporation was generally studied for two different evaporation regimes. The first is a slow drying of a drop in an atmosphere of another non-condensable gas. The evaporation is thus limited by the speed of diffusion of the vapour in the gas.
A stationary spatial distribution of the vapour concentration is assumed. It results in a well-known distribution of $q_i^L$ along the drop interface, see Poulard et al. (2003); Ristenpart et al. (2007) and references therein. The second drop evaporation regime is the opposite limit of the strong evaporation limited by the heat delivery rate. This second regime of evaporation of a 2D sessile (posed on a heater, see Fig. 3) liquid droplet in the atmosphere of its saturated vapour will be solved in order to illustrate the application of the ideas developed above. We use this example simply because it is easier to treat than the bubble growth. The droplet is assumed to be so shallow that the lubrication approximation can be applied to its whole surface. A similar problem has been already considered by Anderson & Davis (1995) in the approximation of isothermal heater and evaporation localised exclusively at the CL. These approximations are dropped here. Among other differences one can list our omission of Marangoni flow by the reasons already discussed (pure fluid) and the assumption of $\theta$ independent of the CL velocity based on more recent results of atomistic simulations of Hadji constantinou (1999). Unlike Anderson & Davis (1995), we do not consider here the wetting hysteresis. Note that it can be accounted for in a natural way by introducing surface heterogeneities modeled with the variation of $\theta$ along the solid surface (Nikolayev 2005).

The particularity of the drop geometry (Fig. 3) consists in the CL position determination. Instead of being determined from the matching of micro and macro regions, it is defined by introducing an additional equation, that for the (2D) drop volume $V$. Its time variation is defined by the global heat balance equation

$$ H \rho_L \frac{dV}{dt} = - \int_{\Omega_{LS}} q_S(x) dx, \quad (5.1) $$

† The assumption of the stationarity leads to the vapour concentration inversely proportional to the distance from the drop. Note that since this function is non-integrable, the heat flux expression based on it is not entirely justified.
Table 1. Dimensional quantities used to make the variables dimensionless.

| Variable              | Notation | Dimensional quantity |
|-----------------------|----------|----------------------|
| length                | $x, h, l_s$ | $d$                  |
| time                  | $t$      | $d^2/\alpha_S$       |
| velocity              | $v^i$    | $\alpha_S/d$         |
| pressure jump         | $\Delta p$ | $\sigma/d$          |
| heat flux             | $q_S$    | $\hat{q} = C\sqrt{\pi\alpha_S}$ |
| interface resistance  | $R_i$    | $d/k_L$              |

where the assumption (3.6) has been applied.

By taking into account the well known expression

$$\frac{dV}{dt} = -\int_{\Omega_{LS}} v^i(x)dx,$$  \hspace{1cm} (5.2)

Eq. (5.1) can be rewritten in the form

$$\int_{\Omega_{LS}} \left[ v^i(x) - \frac{q_S(x)}{\rho_L H} \right] dx = 0 \hspace{1cm} (5.3)$$

more convenient to use in the present context.

The initial shape is chosen separately for each of two problems considered below but the contact angle is always equal to $\theta$. The initial drop height defines the length scale $d$ of the problem.

5.1. Reduction to dimensionless form

The dimensional parameters used as the characteristic scales to reduce the governing equations to the dimensionless form are shown in Table 1 where the flux value $\hat{q}$ used
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for non-dimensionalising purposes can be related to the reference heat flux \( q_{ref} \)

\[
\dot{q} = q_{ref} \left( 1 + \frac{k_S}{k_L} \sqrt{\frac{\alpha_L}{\alpha_S}} \right). \tag{5.4}
\]

Once made dimensionless, the set of equations (3.8, 4.10, 4.15) reduces to

\[
\frac{\dot{\tilde{R}}}{2} \tilde{q}_S(\tilde{x}, \tilde{t}) [\tilde{R}^i + \tilde{h}(\tilde{x}, \tilde{t})] + \frac{N_T}{2} [\Delta \tilde{p}(\tilde{x}, \tilde{t}) - \Delta \tilde{p}_0] = \]

\[
\sqrt{\frac{\tilde{t}}{\pi}} - \int_0^t d\tau \int_{x_{CL}}^{x_{CL}} \tilde{q}_S(x', \tau) g(\tilde{x} - x', \tilde{t} - \tau) dx', \tag{5.5}
\]

\[
\left( \frac{\tilde{h}^3}{3} + \tilde{h}^2 \tilde{L}_s + \beta \tilde{h}^2 \right) \frac{\partial \Delta \tilde{p}}{\partial \tilde{x}} = N_\mu \int_{x_{CL}}^{\tilde{x}} [\tilde{v}(x) - N_q \tilde{q}_S(x')] dx', \tag{5.6}
\]

\[
\frac{\partial^2 \tilde{h}}{\partial \tilde{x}^2} = \Delta \tilde{p} + N_r \tilde{q}_S^2, \tag{5.7}
\]

where

\[
g(x, t) = \frac{1}{4\pi t} \exp \left( -\frac{x^2}{4t} \right) \tag{5.8}
\]

is the Green function for the transient heat conduction problem (Carslaw & Jaeger 1959) and tilde means the corresponding dimensionless parameter. Eq. (3.6) is accounted for in (5.6).

The following dimensionless groups are identified

\[
r = \frac{k_S}{k_L}, \]
\[
Nr = \frac{\tilde{q}^2 d}{\rho v H^2 \sigma}, \]
\[
Nq = \frac{\dot{q} d}{\rho_L H \alpha_S}, \]
\[
N_v = \frac{\sigma}{d \rho_L H}, \]
\[
N_e = \frac{\dot{q} d}{k_S T_{sat}}, \]
\[
N_\mu = \frac{\mu a_S}{\sigma d} \tag{5.9}
\]

\( \tilde{R}^i \) can be seen as an effective dimensionless length scale corresponding to the interfacial thermal resistance. \( N_\mu \) represents the dimensionless viscous relaxation time \((\mu d/\sigma)\). \( N_r \) measures the strength of the vapour recoil relative to the surface tension. The number
$N_q$ shows the contribution of the heat diffusion in terms of the latent heat transport. $N_e$ shows how far the heating drives the system out of thermal equilibrium. And finally, $N_\sigma$ characterises the contribution of the surface tension to the variation of the local interface temperature. $N_T = N_\sigma / N_e$ is introduced in (5.5) for the sake of brevity.

Eqs. (5.6-5.7) should be supplied with the boundary conditions corresponding to (4.16) defined at the CL:

\[
\hat{h} = 0 \quad \text{and} \quad \frac{\partial \hat{h}}{\partial \hat{x}} = \mp \theta \quad \text{at} \quad \hat{x} = \pm \hat{x}_{CL}. \tag{5.10}
\]

The dimensionless equation (5.3) reads

\[
\int_{\hat{x}_{CL}}^{\hat{x}_{CL}} \left[ \tilde{v}^i(x') - N_q \tilde{q}_S(x') \right] dx' = 0. \tag{5.11}
\]

The time evolution of the drop surface is defined by the velocity expression

\[
\tilde{v}^i = -\frac{\partial \hat{h}}{\partial \hat{t}} \tag{5.12}
\]

that follows from (C1).

### 5.2. Symmetry considerations

In the following, the advantage of the drop symmetry will be taken and only a half of the drop $0 < \hat{x} < \hat{x}_{CL}$ will be treated. The integration in (5.5) (5.11) can then be performed over a half of the drop base,

\[
\frac{r}{2} \tilde{q}_S(\hat{x}, \hat{t}) [\tilde{R}^i + \hat{h}(\hat{x}, \hat{t})] + \frac{N_T}{2} [\Delta \hat{p}(\hat{x}, \hat{t}) - \Delta \hat{p}_0] = \\
\sqrt{\frac{\hat{t}}{\pi}} - \int_0^\hat{x}_{CL} d\tau \int_0^\tau \tilde{q}_S(x', \tau) [g(\hat{x} - x', \hat{t} - \tau) + g(\hat{x} + x', \hat{t} - \tau)] dx' ,
\]

\[
\int_{\hat{x}_{CL}}^{\hat{x}_{CL}} [\tilde{v}^i(x') - N_q \tilde{q}_S(x')] dx' = 0. \tag{5.14}
\]

An additional symmetry boundary condition

\[
\frac{\partial \hat{h}}{\partial \hat{x}} = 0 \tag{5.15}
\]
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is necessary to be defined in the drop centre \( \tilde{x} = 0 \) to replace the boundary conditions (5.10) at \( \tilde{x} = -\tilde{x}_{CL} \). The temporal and spatial behaviour of three variables \( \tilde{q}_S, \Delta \tilde{p}, \tilde{h} \) and the temporal variation of \( \tilde{x}_{CL} \) can now be found numerically.

Remark: When one uses the differential form (4.8) of the pressure equation one needs one more boundary condition because of its higher order. The condition

\[
\frac{\partial \Delta \tilde{p}}{\partial \tilde{x}} = 0.
\]

(5.16)

at \( \tilde{x} = 0 \) can be employed. One notices that it follows from the equations (5.6, 5.14).

The dimensionless deviation of \( T_S \) from \( T_{sat} \) defined as

\[
\Delta \tilde{T}_S = \frac{(T_S - T_{sat})}{T_{sat}}
\]

(5.17)
takes the following form according to (3.4, 3.5):

\[
\Delta \tilde{T}_S(\tilde{x}) = \Delta \tilde{p}_0 N_e \sqrt{\frac{\tilde{t}}{\pi}} - 2N_e \int_0^{\tilde{x}_{CL}} \int_0^{\tilde{t}} \tilde{q}_S(x', \tau)[g(\tilde{x} - x', \tilde{t} - \tau) + g(\tilde{x} + x', \tilde{t} - \tau)]dx'.
\]

(5.18)

Once (5.13) is solved and \( \tilde{q}_S(x) \) is known for \( x \in (0, \tilde{x}_{CL}) \), (5.18) allows \( T_S(\tilde{x}) \) to be determined over the whole heater surface \( \tilde{x} \in (0, \infty) \). The alternative expression that follows from (3.7) is valid only for \( x \in (0, \tilde{x}_{CL}) \):

\[
\Delta \tilde{T}_S = \Delta \tilde{p} N_e + N_e r \tilde{q}_S(\tilde{R} + \tilde{h}).
\]

(5.19)

5.3. Numerical implementation

The boundary element method (BEM) can be applied to solve (5.13). Since the problem is non-linear it will be solved by iterations. The interval \( (0, \tilde{x}_{CL}) \) is divided into \( m \) "boundary elements" (BE) and the interval \( (0, \tilde{t}) \) is divided into \( F \) equal subintervals \( \Delta t \) with \( \tilde{t} = F \Delta t \). In principle, \( m \) can be allowed to change with time but in the present example we will keep it constant. Similarly to the BEM described by Nikolayev et al. (2001), the variables are supposed to be constant during each of subintervals and on
each BE. The nodes are chosen in the centres of the BEs. The abscissas of the mesh points (BE’s ends) at the time moment $F$ are denoted $x_i^F$. The abscissa of the $i$-th node and the BE length are denoted respectively $x_{nF}^i = 0.5(x_{i-1}^F + x_i^F)$ and $d_i^F = x_i^F - x_{i-1}^F$.

The interval $(0, \tilde{x}_{CL})$ is remeshed at each time step because of the moving boundary.

The $\tilde{q}_S$ value of at $j$-th node and during $f$-th time step is denoted $q_{fj}$. The corresponding values of $\Delta \tilde{p}$ and $\tilde{h}$ are denoted respectively $p_{jf}$ and $h_{jf}$. The discrete analog of (5.13), that holds for $i = 1 \ldots m$ is

$$
\frac{r}{2} q_i^F \left[ \tilde{R}_i^F + h_i^F(p - \Delta \tilde{p}_0) \right] + \frac{N_r}{2} (p_i^F - \Delta \tilde{p}_0) = \sqrt{\frac{F \Delta t}{\pi}} - \sum_{f=1}^{F} \sum_{j=1}^{m} G_{ij}^{F} q_{jf}^F, \quad (5.20)
$$

where the value at the previous iteration is denoted with the upper index $pre$. The symmetrised “coefficients of influence” are defined by the expressions

$$
G_{ij}^{F} = \int_{x_{i-1}^{F}}^{x_i^{F}} dx \int_{(j-1)\Delta t}^{j\Delta t} [g(x_{nF}^i - x, F\Delta t - \tau) + g(x_{nF}^i + x, F\Delta t - \tau)] d\tau
$$

$$
= \chi_{ij}^{F}(x_{j-1}^{F} - x_{nF}^i) - \chi_{ij}^{F}(x_j^{F} - x_{nF}^i)
$$

$$
= \chi_{ij}^{F}(x_{j-1}^{F} + x_{nF}^i) - \chi_{ij}^{F}(x_j^{F} + x_{nF}^i),
$$

(5.21)

The coefficient $\chi$ can be found analytically:

$$
\chi_{ij}^{F}(x) = f_{\chi} [x, (F - f + 1)\Delta t] - f_{\chi} [x, (F - f)\Delta t], \quad (5.23)
$$

where

$$
f_{\chi}(x, t) = \frac{1}{4\sqrt{\pi}} \left[ 2\sqrt{t} \text{erfc} \left( \frac{x}{2\sqrt{t}} \right) - \frac{x}{\sqrt{\pi}} E_1 \left( \frac{x^2}{4t} \right) \right],
$$

and $\text{erfc}(\cdot)$ and $E_1(\cdot)$ are the complementary error function and the exponential integral respectively (Abramovitz & Stegun 1972). Note that $\chi_{ij}^{F}(x) = f_{\chi}(x, \Delta t)$.

The remaining equations (5.6, 5.7) are discretised using the finite volume method (FVM) (Patankar 1980). The discretised first order equation (5.6) is written for $i =$
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\[
p_{i+1}^F - p_i^F = N \mu \sum_{j=i}^{m} d_j^F \left[ \frac{x_j^{nF} - x_j^{n(F-1)}}{\Delta t} u_j^{F-1} - \frac{h_j^F - h_j^{F-1}}{\Delta t} - N_q j^F \right], \tag{5.24}
\]

where

\[
a_i = \frac{d_i^F}{2h_i^{F(pre)} \left\{ \left[ h_i^{F(pre)} \right]^2 / 3 + h_i^{F(pre)} l_s + \beta l_s^2 \right\}}
\]

and the formula (C.5) was employed. The discretised second order Eq. (5.7) holds for \( i = 2, \ldots, (m-1) \). It reads

\[
\frac{h_i^{F+1} - h_i^F}{x_i^{nF+1} - x_i^{nF}} - \frac{h_i^F - h_i^{F-1}}{x_i^{nF} - x_i^{nF-1}} = d_i^F \left\{ p_i^F + N_r \left[ q_i^{F(pre)} \right]^2 \right\}.
\]

Accordingly to the order of the equations, three boundary conditions (5.10, 5.15) are needed:

\[
h_{m}^F = -\theta (x_m^F - x_m^{nF}), \tag{5.26}
\]

\[
\frac{h_1^F - h_1^F}{x_1^{nF} - x_1^{nF}} = d_1^F \left\{ p_1^F + N_r \left[ q_1^{F(pre)} \right]^2 \right\}, \tag{5.27}
\]

\[
-\theta - \frac{h_m^F - h_{m-1}^F}{x_m^{nF} - x_{m-1}^{nF}} = d_m^F \left\{ p_m^F + N_r \left[ q_m^{F(pre)} \right]^2 \right\}.
\]

The contact line position \( x_m^F \) at time step \( F \) is found by solving the equation (5.14)

\[
\sum_{j=1}^{m} d_j^F \left[ \frac{x_j^{nF} - x_j^{n(F-1)}}{\Delta t} u_j^{F-1} - \frac{h_j^F - h_j^{F-1}}{\Delta t} - N_q j^F \right] = 0 \tag{5.29}
\]

with Newton’s algorithm. The material parameters for water at 10 MPa on the stainless steel (Table 2) are used for the calculations. The equilibrium contact angle is assumed to be \( \theta = 5^\circ \). The slip length value is uncertain. According to the detailed analysis of Langa et al. (2007), its value varies from 1 nm to 1 \( \mu \)m depending on wettability and the state of the solid surface. Unless mentioned specifically, \( l_s = 10 \) nm value is adopted.

5.4. Isothermal drop retraction

First, one needs to check if the second derivative boundary condition gives reasonable results. We perform here only a brief check. Detailed comparison with existing experimen-
| Description                              | Notation | Value | Units  |
|------------------------------------------|----------|-------|--------|
| Saturation temperature                   | $T_{\text{sat}}$ | 311   | $^\circ$C |
| Thermal conductivity of liquid           | $k_L$    | 0.55  | W/(m K) |
| Specific heat of liquid                  | $c_{pL}$ | 6.12  | J/(g K) |
| Mass density of liquid                   | $\rho_L$ | 688.63| kg/m$^3$ |
| Mass density of vapor                    | $\rho_V$ | 55.48 | kg/m$^3$ |
| Latent heat of vaporization              | $H$      | 1.3   | MJ/kg  |
| Surface tension                          | $\sigma$ | 12.04 | mN/m   |
| Thermal conductivity of steel            | $k_S$    | 15    | W/(m K) |
| Specific heat of steel                   | —        | 0.5   | J/(g K) |
| Mass density of steel                    | —        | 8000  | kg/m$^3$ |

Table 2. Material parameters used in the simulation.

data will be made elsewhere. As a test problem, we use the classical drop retraction problem which consists in solving the hydrodynamic part of the problem, eqs. (5.24-5.29), in which the heat fluxes $q_i^c$ are zeroed and the drop volume remains constant throughout the evolution.

Initially, a pancake drop shape is chosen. It is supposed to relax to the final circular shape. The drop shape evolution is presented in Fig. 4a. Fig. 5 shows the evolution of the contact line position. The influence of the slip length on the CL dynamics is shown. It is evident that $l_s$ controls the CL relaxation rate: the smaller $l_s$ the slower is the CL motion.

As mentioned in the previous section, both Navier and second derivative slip conditions may be applied for the isothermal problem. The influence of the boundary condition on the CL dynamics is shown for $l_s = 10$ nm. The behaviour is similar although the Navier
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Figure 4. Dynamics during drop retraction at constant volume (no evaporation). (a) Drop shape evolution obtained with the second derivative boundary condition (4.7). The arrows show the shape evolution directions. Note the difference of length scales on x and y axes. (b) Spatial variation of the pressure jump $\Delta p$ in the semi-log coordinates for the second derivative ($\beta = 0.5$) and Navier ($\beta = 0$) slip conditions. One notes the pressure finiteness and divergence in the former and latter cases, respectively. The influence of the discretisation ($d_{\text{min}}$ is the minimal grid size) on the results is also shown.

Condition results in a slightly slower contact line motion than the second derivative condition. The difference in the pressure behaviour is however much stronger. Fig. 4.b shows a typical spatial variation of the pressure jump. It remains negative along the whole drop contour and decreases near the contact line which corresponds to the growing by absolute value curvature and the apparent contact angle smaller than $\theta$ which is a usual feature of the receding CL motion without evaporation (Snoeijer et al. 2007). Comparing to the Navier condition case, the second derivative condition results in a smaller variation of the pressure in agreement with the asymptotic analysis carried out in sec. 4.1. The results of the stability of the numerical algorithm with respect to the spatial meshing are also shown. One notices that the grid refinement leads to strong correction of the CL pressure for the Navier case, while this correction is negligible for the second derivative condition case where the pressure is bounded. In practice this means that the stability
Figure 5. Contact line dynamics in isothermal case. Comparison of the evolutions obtained with the Navier and second derivative slip conditions calculated for the same slip length and the influence of the slip length on the contact line dynamics within the second derivative slip model.

The performance of the numerical algorithm is much better for the second derivative condition than for the Navier condition.

5.5. Drop evaporation with retraction

It is well known that there are two regimes of drop evaporation: with and without CL retraction. The regime of immobile contact line occurs due to its pinning on the solid surface defects and will not be considered in this paper.

The solution of the full problem taking the evaporation into account results typically in the drop surface evolution shown in Fig. 6. The drop is initially has an equilibrium shape corresponding to the contact angle $\theta = 5^\circ$. The initial pressure jump $\Delta p_0$ is chosen accordingly to the drop initial curvature, Eq. 4.11. Than the bulk heating of the solid begins and the drop volume decreases until the drop evaporates completely, see Fig. 7.

One mentions several features of this evolution. While the drop volume decreases almost linearly, the time evolution of other parameters is more sophisticated. Instead of a monotonous decrease that one would expects, the drop height grows about 30% before starting to decrease. This occurs because of the impulse heating mode chosen here.
Figure 6. Dynamics during the drop evaporation. (a) Drop shape evolution for $q_{ref} = 0.5\text{W/cm}^2$. The arrows show the shape evolution directions. The shape in the CL vicinity for $t = 21.34\text{ ms}$ (marked approximately with a small rectangle) is zoomed in the insert in the upper right corner of the plot where the circles show the calculated interface and the straight line indicates the asymptote at the CL. (b) Evolution of the contact line position for two different values of $q_{ref}$.

Figure 7. Time evolution of the drop volume and height for $q_{ref} = 0.5\text{W/cm}^2$.

Because of the high heat input in the beginning of the evolution, the heat flux attains rapidly high values at the CL (Fig. 8b). The difference of heat fluxes at the CL and at the top of the drop is especially high in the beginning of the evolution. High heat flux means high velocity of the fluid supply causing a high pressure drop at the CL reflected in Fig. 8a. The interface curvature is defined mainly by the pressure jump since
the vapour recoil contribution is small in the range of the heat fluxes considered in the simulation. Therefore the curvature in the vicinity of the CL follows almost instantaneously the heating impulsion. Since the curvature defines the rate of spatial change of the interface slope, a high curvature means that the apparent (visible) contact angle becomes larger than $\theta$. This feature is visible in Fig. 6a, where the actual contact angle is always equal to $\theta$. However the apparent contact angle increases right from the beginning of the evolution. Note that the vapour recoil term also leads to the apparent contact angle increase as described in detail by Nikolayev & Beysens (1999); the effect thus should become even stronger at higher heat fluxes. The time variation of the volume is relatively slow because it follows the averaged over the drop surface heat flux. It is evident that the increase of the apparent contact angle at almost fixed volume should result in the initial increase of $h_{max}$ (Fig. 7). This effect should exist as well in 3D and can thus be observed experimentally. Although the apparent contact angle increase during evaporation is predicted by many approaches (Wayner et al. 1976; Hocking 1995; Anderson & Davis 1995) and has been observed by Poulard et al. (2003); Hegseth et al. (2005) among many others, the height “jump” at impulse heating was not studied experimentally.

Accordingly to this picture, two stages of drop evaporation can be identified in Figs. 6 and 7. First, the CL moves fast (Fig. 6b, $t \lesssim 7$ ms for $q_{ref} = 0.5 \text{W/cm}^2$), the apparent contact angle and the drop height grow. On the second stage ($t \gtrsim 7$ ms), the apparent contact angle stabilises, $h_{max}$ starts to decrease and the CL receding speed becomes smaller.

As a matter of fact, the evaporation and interface velocity terms enter the r.h.s. of the pressure equation (4.10) with the opposite signs. On one hand, a positive interface velocity leads to the reduction of curvature (like in the drop retraction problem, Fig. 4b). On the other hand, the evaporation causes the curvature increase and it is difficult
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Figure 8. (a) Pressure jump and (b) heat flux across the vapour-liquid interface versus distance to the contact line in semi-log and log-log coordinates respectively for $q_{ref} = 0.5\,\text{W/cm}^2$.

to predict the pressure behaviour a priori. Fig. 8a shows that the latter tendency wins. One can see in Fig. 8a that the curvature near the CL can become orders of value larger than in the centre of the drop. In addition, the pressures in the drop centre and at the CL are of the opposite signs so that an inflection point exists. It is not resolved in the drop shapes of Fig. 6a because it is situated at less than 1 $\mu\text{m}$ from the CL according to Fig. 8a. The positive curvature and the appearance of the large apparent contact angle is illustrated in the insert to Fig. 6a where a close vicinity of the CL is presented. Note that the pressure is finite at the CL as it should be according to the asymptotic analysis of sec. 4.1.

Another interesting feature already underlined in many studies [Stephan & Hammer 1985; Anderson & Davis 1995; Nikolayev et al. 2001] is the localisation of the heat and mass transfer in a close vicinity of the CL. Fig. 8b shows that the almost all heat flux (and thus evaporation) is concentrated on about 1% of the vapour-liquid interface in a close vicinity of the CL. Note that unlike the calculation involving the adsorption film...
Figure 9. Snapshots of the temperature variation along the heater surface for $q_{ref} = 0.5\text{W/cm}^2$.

Note the sharp minimum appearing in the close vicinity of the CL. The times corresponding to the curves are given in ms.

(Wayner et al. 1976; Stephan & Hammer 1985), the heat flux does not vanish at the CL and attains there its maximum. The discontinuity of $q_S(x)$ thus occurs at the CL.

The variation of the temperature (5.18) along the whole heater surface presented in Fig. 9 reflects this discontinuity. At small heat fluxes considered here, the absolute variation of the heater surface superheating defined as $T_S - T_{sat}$ is of the order of 0.5 K at this heat flux. $T_S$ exhibits a minimum at the CL due to the strong latent heat consumption. The minimum is very sharp and corresponds to the locally high heat exchange along the heating surface so the temperature gradients are huge in this area and correspond to the high heat flux $q_L^i$ (Fig. 8b). This explains why the temperature variation along the heater needs to be accounted for. The sharp temperature minimum at the CL has been obtained both in simulations (see e. g. Nikolayev et al. (2001)) and experiments (see e. g. Theophanous et al. (2002)) both for drop evaporation and bubble growth in boiling.

The results of this section have been obtained using the second derivative boundary condition (4.7). One needs to mention that the case of Navier slip condition could in principle be treated numerically. However it would result in the dependence of the results on the spatial discretisation because of the pressure singularity.
6. Conclusions

The adsorption (or prewetting) liquid film that has been assumed to cover continuously the heater in prior studies of the liquid meniscus evaporation. On the heated surfaces, its thickness is found to be smaller than few nanometres under practically important conditions. Since the fluid flow in such films is insignificant, the true triple liquid-vapour-heater contact needs to be considered.

Two major difficulties occur while describing the heat and fluid flow in the vicinity of the contact line, namely the thermal and hydrodynamic singularities that need to be relaxed. The hydrodynamic singularity is especially important because the Navier slip boundary condition used conventionally for its relaxation turns out to be inappropriate when evaporation/condensation is involved. While the viscous stresses are relaxed with the Navier slip condition, the pressure remains infinite and causes a non-physical divergence of temperature at the contact line. Another, “second derivative” slip condition is proposed. It relaxes both viscous stress and pressure singularities. We show that for the conventional dynamic contact line problems with no heat transfer it results in a behaviour very similar to that obtained with the Navier slip condition.

High heat fluxes occurring at the contact line create important temperature gradients even in the metal heaters with high heat conductivity. This requires considering the heat conduction in the heater. Because of fast change in geometry due to the moving contact line, the transient heat conduction in the heater needs to be solved.

On one hand, the shape of the vapour-liquid interface changes in time because of the action of various forces. This shape change induces a non-stationary flow in the bulk of the liquid. On the other hand, the interfacial evaporation (condensation) creates another flow bringing the liquid to the interface. These both flows are coupled and determine the contact line position.
An approach describing the contact line motion caused by evaporation (or possibly condensation) and integrating all the ingredients mentioned above has been developed by using the lubrication approximation. It allows solving of the conjugate problems of hydrodynamics and heat transfer (liquid and solid domains) in the “microregion”, a vicinity of the contact line where the main part of the heat and mass transfer takes place. This approach can be used to describe many practical situations like bubble dynamics during the boiling, drop evaporation or condensation etc.

A problem of evaporation of a 2D drop posed on a heated support in the atmosphere of saturated vapour has been considered and analysed under assumption of the ideally smooth surface (no pinning). Due to the impulse mode of heating, a brief height increase of the drop occurs in spite of the drop volume decrease. This effect is a manifestation of the localisation of the evaporation at the contact line and associated with the apparent contact angle increase.

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Appendix A. Lubrication theory for the moving contact line with heat and mass transfer

The lubrication theory has been developed independently by Petroff (1883) and Reynolds (1886). The case of simultaneous heat and mass transfer has been treated in several papers (see e.g. Hocking (1995); Anderson & Davis (1995)). However, the lubrication equations were written there in somewhat different form inconvenient for the purposes of the present study. For the convenience of the Reader, the employed equations are re-derived here.
For thin fluid layers, the fluid is supposed to move mainly along $x$ axis (Fig. 2), i.e. $v_x \gg v_y$. In addition, the $v_x$ variation across the layer is assumed to be much larger than along it: $\partial v_x/\partial y \gg \partial v_x/\partial x$. The Stokes equations then reduce to:

$$
\frac{\partial p_L}{\partial x} = \mu \frac{\partial^2 v_x}{\partial y^2}, \quad (A 1)
$$
$$
\frac{\partial p_L}{\partial y} = 0. \quad (A 2)
$$

By taking the $y$ derivative of (A 1) and using (A 2) one arrives at the equation $\partial^3 v_x/\partial y^3 = 0$, the solution of which is

$$
v_x = a + by + cy^2, \quad (A 3)
$$

where $a, b, c$ are independent of $y$. They are to be determined from the boundary conditions. The first of them reflects the absence of the tangential stresses at the free vapour-liquid interface $y = h(x)$

$$
\frac{\partial v_x}{\partial y} = 0. \quad (A 4)
$$

The volume flux $Q$ flowing through the film at a given position $x$

$$
Q = \int_0^h v_x(y) dy \quad (A 5)
$$

serves as the second equation for three unknowns $a, b, c$. The third condition is given by either (4.2) or (4.7). The back substitution of the solution into (A 1) written at the vapour-liquid interface results in the following expressions:

$$
Q = -\frac{1}{\mu} \left( \frac{h^3}{3} + h^2 l_s \right) \frac{\partial p_L}{\partial x} \quad (A 6)
$$

and

$$
Q = -\frac{1}{\mu} \left( \frac{h^3}{3} + h^2 l_s + h \beta l_s^2 \right) \frac{\partial p_L}{\partial x} \quad (A 7)
$$

written for the boundary conditions (4.2) and (4.7) respectively.

By using the fluid mass conservation, $Q$ can also be expressed via the component $v_n$.
of the liquid velocity normal to the vapour-liquid interface:

\[ Q = \int_0^l v_n(l)dl \approx \int_{x_{CL}}^x v_n(x)dx. \]  
\[(A \, 8)\]

\[(A \, 8)\] can be rewritten as

\[ v_n = \frac{\partial Q}{\partial x}, \]  
\[(A \, 9)\]

where \( v_n \) is related to the heat flux at the interface \( q_L^i \) (assumed positive when the heat flows from the liquid side, i.e. at evaporation) known from the heat transfer problem via the mass conservation law

\[ \eta = (v^i - v_n)\rho_L = q_L^i / H. \]  
\[(A \, 10)\]

The normal interface velocity \( v^i \) is considered to be positive if directed inside the liquid (as the vector \( \vec{n} \) in Fig. 2). It is assumed here that the heat conduction in the vapour is negligible with respect to that in the liquid.

By injecting \[(A \, 10)\] and \[(A \, 6)\] or \[(A \, 7)\] into \[(A \, 9)\], one arrives finally to the expressions \[(4.3)\] or \[(4.10)\] obtained with \[(4.2)\] or \[(4.7)\] respectively.

**Appendix B. Asymptotic analysis for the nonlinear slip boundary condition**

A nonlinear power slip law

\[ v_x = \varepsilon \left( \frac{\partial v_x}{\partial y} \right)^\gamma \]  
\[(B \, 1)\]

that generalises \[(4.2)\] is applied here in the asymptotic limit \( x \to x_{CL} \) where \( \gamma \) is some power. By repeating the procedure described in Appendix A, one obtains easily the equation

\[ Q = h \varepsilon \left( \frac{h}{\mu} \frac{\partial \Delta p}{\partial x} \right)^\gamma + \frac{h^3}{3\mu} \frac{\partial \Delta p}{\partial x}. \]  
\[(B \, 2)\]
One can reuse the argument that led to (4.5) and get instead an asymptotic expression
\[ \varepsilon \left( \frac{h \partial \Delta p}{\mu \partial x} \right)^\gamma + \frac{h^2 \partial \Delta p}{3\mu \partial x} \sim \text{const.} \]  
(B3)

Let us now consider the terms in the l.h.s. If the second of them was prevailing at \( x \to x_{CL} \), the divergence would be non-integrable like in the case of no-slip condition. Therefore, the first term must be prevailing. The second term can then be neglected and it becomes evident that (B3) results in (4.6) independently of the value of \( \gamma \).

Appendix C. Numerical calculation of the velocity of the moving interface

Calculation of the normal velocity of the interface from the time evolution of the interface shape is somewhat delicate. The expression
\[ v^i = -\frac{\partial h}{\partial t} (1 + u^2)^{-1/2} \approx -\frac{\partial h}{\partial t}. \]  
(C1)

commonly used in the standard lubrication theory (see e.g. Hocking (1995)) requires that \( x \) is maintained constant while calculating the time derivative. For the calculation purposes, this derivative needs to be replaced by the finite difference
\[ \left. \frac{\partial h}{\partial t} \right|_{x=x_i^{n_F}} \simeq \frac{h^F(x=x_i^{n_F}) - h^{F-1}(x=x_i^{n_F})}{\Delta t}, \]  
(C2)

where the superscript means the time step number and the subscript enumerates the grid points. Eq. (C2) involves the height of the interface \( h^{F-1} \) defined at a grid position \( x_i^{n_F} \) at the next time step. Since the grid points move when the interface moves, one would need to interpolate in order to find \( h^{F-1} \) at \( x = x_i^{n_F} \) because \( h^{F-1} \) is known only at the node points \( x_i^{n(F-1)} \). In addition, the contact line motion can make impossible finding of \( h^{F-1}(x = x_i^{n_F}) \) if \( x_{CL}^{F-1} < x_i^{n_F} < x_{CL}^F \), i.e. if the interface at time \( F - 1 \) did not exist at \( x = x_i^{n_F} \). Both these difficulties can be avoided if the expression for the full derivative of
\[ \frac{dh}{dt} = \frac{dx^i}{dt} \frac{\partial h}{\partial x^i} + \frac{\partial h}{\partial t} \] (C 3)

is applied. Its finite difference approximation is easy to calculate,

\[ \left. \frac{dh}{dt} \right|_{x=x^n} \approx \frac{h^F(x=x^n) - h^{F-1}(x=x^{n(F-1)})}{\Delta t} \equiv \frac{h_i^F - h_{i-1}^{F-1}}{\Delta t}. \] (C 4)

By using this expression, one obtains

\[ v_i(x = x^n) \approx \frac{x_i^{nF} - x_{i}^{n(F-1)}}{\Delta t} \alpha_{i}^{F-1} - \frac{h_i^F - h_{i-1}^{F-1}}{\Delta t} \] (C 5)

and both above mentioned difficulties are avoided.

REFERENCES

Abramovitz, M. & Stegun, I. A. 1972 *Handbook of Mathematical Functions*. New York.

Ajaev, V. S., Homsy, G. M. & Morris, S. J. S. 2002 Dynamic response of geometrically constrained vapor bubbles. *J. Colloid Interf. Sci.* **254** (2), 346 – 354.

Anderson, D. M. & Davis, S. H. 1995 The spreading of volatile liquid droplets on heated surfaces. *Phys. Fluids* **7**, 248 – 265.

Bartes, M., Reynard, C., Santini, R. & Tadrist, L. 2007 Non-condensable gas influence on the Marangoni convection during a single vapour bubble growth in a subcooled liquid. *Europhysics Lett.* **77**, 14001.

Brochard-Wyart, F., Di Meglio, J.-M., Quere, D. & de Gennes, P.-G. 1991 Spreading of nonvolatile liquids in a continuum picture. *Langmuir* **7** (2), 335 – 338.

Carslaw, H. S. & Jaeger, J. C. 1959 *Conduction of Heat in Solids*, 2nd edn. Oxford: University Press.

Consolini, L., Aggarwal, S. K. & Murad, S. 2003 A molecular dynamics simulation of droplet evaporation. *Int. J. Heat Mass Transfer* **46**, 3179 – 3188.

Cooper, M. G. & Lloyd, A. J. P. 1969 The microlayer in nucleate pool boiling. *Int. J. Heat Mass Transfer* **12**, 895 – 913.

Freund, J. B. 2005 The atomic detail of an evaporating meniscus. *Phys. Fluids* **17**, 022104.
Hadjiconstantinou, N. G. 1999 Combining atomistic and continuum simulations of contact-line motion. *Phys. Rev. E* 59, 2475 – 2478.

Hadjiconstantinou, N. G. 2003 Comment on Cercignani’s second-order slip coefficient. *Physics of Fluids* 15 (8), 2352 – 2354.

Hegseth, J., Oprisan, A., Garrabos, Y., Nikolayev, V. S., Lecoutre-Chabot, C. & Beysens, D. 2005 Wetting film dynamics during evaporation under weightlessness in a near-critical fluid. *Phys. Rev. E* 72, 031602.

Hocking, L. M. 1995 On contact angles in evaporating liquids. *Phys. Fluids* 7, 2950 – 2955.

Israelachvili, J. N. 1992 *Intermolecular and Surface Forces*, 2nd edn. London: Academic Press.

Kern, J. & Stephan, P. 2003 Theoretical model for nucleate boiling heat and mass transfer of binary mixtures. *J. Heat Transfer (Trans. ASME)* 125, 1106 – 1115.

Lauga, E., Brenner, M. P. & Stone, H. A. 2007 Microfluidics: The no-slip boundary condition. In *Springer Handbook of Experimental Fluid Dynamics* (ed. C. Tropea, A. Yarin & J. Foss), chap. 19, pp. 1217 – 1240. New York: Springer, available at: http://maeresearch.ucsd.edu/lauga/references/LBS07_chapter_19.pdf.

Lockerby, D. A., Reese, J. M., Emerson, D. R. & Barber, R. W. 2004 Velocity boundary condition at solid walls in rarefied gas calculations. *Phys. Rev. E* 70 (1), 017303.

Marek, R. & Straub, J. 2001 The origin of thermocapillary convection in subcooled nucleate pool boiling. *Int. J. Heat Mass Transfer* 44, 619 – 632.

Maruyama, S. & Kimura, T. 2000 A molecular dynamics simulation of a bubble nucleation on solid surface. *Int. J. Heat Technology* 18, *supplement* 1, 69 – 74.

Mathieu, B., Lebaigue, O. & Tadrist, L. 2002 Numerical investigation of a dynamic contact line model for perfectly wetting liquids on a heated wall of finite conductivity. In *Proc. 12th Int. Heat Transfer Conf.*, 19-23/8 2002. Grenoble, paper 2468.

Maurer, J., Tabeling, P., Joseph, P. & Willaime, H. 2003 Second-order slip laws in microchannels for helium and nitrogen. *Phys. Fluids* 15 (9), 2613 – 2621.

Morris, S. J. S. 2000 A phenomenological model for the contact region of an evaporating meniscus on a superheated slab. *J. Fluid Mech.* 411, 59 – 89.
NIKOLAYEV, V. S. 2005 Dynamics and depinning of the triple contact line in the presence of periodic surface defects. *J. Phys. Cond. Matt.* **17** (13), 2111 – 2119.

NIKOLAYEV, V. S. & BEYSENS, D. A. 1999 Boiling crisis and non-equilibrium drying transition. *Europhysics Lett.* **47** (3), 345 – 351.

NIKOLAYEV, V. S., BEYSENS, D. A., LAGIER, G.-L. & HEGSETH, J. 2001 Growth of a dry spot under a vapor bubble at high heat flux and high pressure. *Int. J. Heat Mass Transfer* **44** (18), 3499 – 3511.

NIKOLAYEV, V. S., CHATAIN, D., GARRABOS, Y. & BEYSENS, D. 2006 Experimental evidence of the vapor recoil mechanism in the boiling crisis. *Phys. Rev. Lett.* **97**, 184503.

van OUWERKERK, H. J. 1972 Burnout in pool boiling: the stability of boiling mechanisms. *Int. J. Heat Mass Transfer* **15**, 25 – 34.

PATANKAR, S. V. 1980 *Numerical heat transfer and fluid flow*. Washington: Hemisphere.

PETROFF, N. P. 1883 Friction in machines and the effect of lubricant. *Inzhenernyj Zhurnal, Sankt-Peterburg* **1-4**, 71 – 140, 228 – 279, 377 – 436 and 535 – 564, published in four issues.

Poulard, C., Bénichou, O. & Cazabat, A. M. 2003 Freely receding evaporating droplets. *Langmuir* **19** (21), 8828 – 8834.

REYNOLDS, O. 1886 On the theory of lubrication and its application to Mr Beauchamp Tower’s experiments, including an experimental determination of viscosity of olive oil. *Phil. Trans.* **177**, 157 – 234.

RISTENPART, W. D., KIM, P. G., DOMINGUES, C., WAN, J. & STONE, H. A. 2007 Influence of substrate conductivity on circulation reversal in evaporating drops. *Phys. Rev. Lett.* **99** (23).

SHIKHMURZAEV, Yu. D. 1997 Spreading of droplets on solids in quasi-static regime. *Phys. Fluids* **9**, 266 – 275.

SNOELIER, J., ANDREOTTI, B., DELON, G. & FERMIGIER, M. 2007 Relaxation of a dewetting contact line. Part 1. A full-scale hydrodynamic calculation. *J. Fluid Mech.* **579**, 63 – 83.

SON, G. & DHIR, V. K. 1999 Dynamics and heat transfer associated with a single bubble during nucleate boiling on a horizontal surface. *J. Heat Transfer (Trans. ASME)* **121**, 623 – 631.
Dynamics of the triple contact line on the non-isothermal heater

Stephan, P. & Hammer, J. 1985 A new model for nucleate boiling heat transfer. *Wärme- und Stoffübertragung* **30**, 119 – 125.

Theophanous, T. G., Dinh, T. H., Tu, J. P. & Dinh, A. P. 2002 The boiling crisis phenomenon. Part II: Dryout dynamics and burnout. *Exp. Thermal Fluid Sci.* **26**, 793 – 810.

Torikai, K., Suzuki, K. & Yamaguchi, M. 1991 Study on contact area of pool boiling bubbles on a heating surface. *JSME Int. J. Series II* **34**, 195 – 199.

Wayner, P. C., Kao, Y. K. & LaCroix, L. V. 1976 The interline heat-transfer coefficient of an evaporating wetting film. *Int. J. Heat Mass Transfer* **19**, 487 – 492.