A HYDRODYNAMIC MODEL WITH LOCAL MARANGONI EFFECTS ARISING FROM MICROFLUIDICS

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Abstract. The aim of the paper is the mathematical and numerical analysis of a contact line dynamics model. The model studied derives from [14]. It is supposed to describe the main features of the advancing triple line: rolling motion and variable contact angle. The model is a coupling between: i) a Navier-Stokes free surface flow with local slip type boundary condition with surface tension gradients and ii) a mesoscopic local surface model giving the surface tension distribution.

A mathematical and numerical analysis of the 1D steady-state local surface model are done. Some 1D numerical computations are performed and lead to a qualitative description of the solution behavior. Then, configurations of a tape plunging into a liquid pool are considered. Given a local surface tension gradient source term - solution of the 1D model-, 2D Navier-Stokes finite element computations show the local Marangoni term influence on the flow. Navier-Stokes flow is solved using an ALE formulation and characteristics methods.
1 INTRODUCTION

The physical phenomena of dynamical contact line appears in many industrial processes such as coating of solids by liquids. Two main features of such viscous and slow flows revealed by experiments are the following: i) the liquid front advances following a rolling motion, similar to a caterpillar vehicle, see [5]: the particles of the liquid-gas interface arrive at the solid-liquid interface; ii) the dynamical contact angle derives from its static value -determined by the classical Young equation-, and depends on the fluid velocity in the bulk. In addition, it seems that its value cannot be prescribed explicitly in a general way, see [1] and the references cited therein for a more complete review.

The contact angle and the triple line velocity are ones of the most important parameter to describe the motion of such flows. The mathematical modeling of the moving contact line is delicate. A no-slip boundary condition at the solid-liquid interface implies a non-physical singularity: the fluid exerts an infinite force on the solid surface, [5]. Then, most of the theories and most of models have been based on a slippage description, see e.g. [9, 6, 3], see also [4, 14] for a more complete review.

A slip condition removes the singularity, however, it replaces the rolling motion by a sliding one, [6]. For a normal liquid flowing over a smooth solid, slippage is usually negligible, [4].

The mathematical model studied in the present paper is derived from those established in [14, 1]. It is supposed to describe the main features of the advancing contact line and to remove the singularity.

The main idea of this model is the following. The rolling motion induces a local variation of the surface tension. This variation would be due to fluid particles going from the liquid-gas interface to the liquid-solid one, [14]. The surface tension gradient induced, influences the motion and the force near the contact line, and implies a Marangoni effect. In this model, the (dynamic) wetting angle is not imposed but is a response of the model.

The paper is organized as follows. In next section, we present the model considered. It is derived from the Shikhmurzaev’s model established in [14, 1]. In section 3, we present a mathematical analysis of the 1D steady-state local surface model. Existence and uniqueness of the solution are proved, also a monotony property is proved. A numerical analysis of the finite element discretization is done. Finally, 1D numerical tests are performed and lead to a qualitative behavior of the local surface tension gradient. In section 4, ALE formulation of the 2D Navier-Stokes model is presented. Then, numerical results are performed using the previous 1D local surface model solution as source term. Test case is a solid tape plunging into a liquid pool at speed $U_s$.

2 THE MATHEMATICAL MODEL

In this section, we consider the configuration of a solid tape plunging vertically into a 2D pool of liquid at speed $U_s$, Fig. 2, and we present a model derived from [14, 1].
We denote by $\Omega$ the liquid pool wetting the solid tape $(S)$, by $\Gamma_{SL}$ the solid-liquid contact surface, by $\Gamma_{SG}$ the solid-gas contact surface, by $\Gamma_{LG}$ the free surface liquid-gas and by $P_{C}$ the contact point liquid-gas-solid.

When the liquid is at rest, the (static) contact angle $\theta_s$ satisfies the classical Young equation: $\sigma_{LG}^{eq} \cos(\theta_s) = \sigma_{SL}^{eq} = \sigma_{SL}^{eq}$, where $\sigma_{LG}^{eq}$, $\sigma_{SL}^{eq}$ and $\sigma_{SG}^{eq}$ are the equilibrium surface tensions of the liquid-gas, solid-liquid and solid-gas interfaces respectively. In this paper, we consider the dynamic case i.e when the solid plate is moving at speed $U_S$. In that case, the contact angle becomes variable. The base of the model studied is to consider that the Young equation remains valid:

$$\sigma_{LG} \cos(\theta_d) = \sigma_{SG} - \sigma_{SL}$$

where $\theta_d$ denotes the dynamic contact angle.

Briefly, the full model considered can be described as follows. A macroscopic Hydrodynamic Free Surface Model -HFSM-, for the fluid motion is coupled to a mesoscopic Local Surface Model -LSM- describing the local surface tension distribution and the contact line motion. The HFSM consists to the Navier-Stokes equations with free surface and slip type boundary conditions. The coupling with the LSM is done through these boundary conditions imposed on a small vicinity of the triple line. The LSM describes the dependence between the surface tension parameters and the fluid motion.
2.1 The macroscopic Hydrodynamic Free Surface Model

We denote by \( \tilde{u} \) the fluid velocity, \( p \) its pressure, \( \Sigma \) the stress tensor, \( \Sigma_{ij} = -p \delta_{ij} + \mu (\partial_i u_j + \partial_j u_i) \) for \( 1 \leq i, j \leq 2 \), where \( \mu \) is the dynamic viscosity. We denote by \(( \tilde{r}, \tilde{n} )\) the unit tangential and external normal vectors such that it is direct. We set \( \Sigma_n = \Sigma . \tilde{n} \in \mathbb{R}^2 \); \( \Sigma_r = \Sigma_n . \tilde{n} + \Sigma_r . \tilde{r} \).

The fluid motion is governed by the incompressible Navier-Stokes equations:

\[
\begin{align*}
\dot{\rho} \frac{\partial u}{\partial t} - (\nabla \Sigma) + \rho (\tilde{u} \cdot \nabla) u_i &= \dot{\rho} g_i & \text{in } (0, T) \times \Omega & 1 \leq i \leq 2 \\
\nabla \cdot u &= 0 & \text{in } (0, T) \times \Omega 
\end{align*}
\]

(2)

where \( \dot{\rho} \) is the fluid density, \( \dot{\rho} \) the gravity, \( T \) the final time and \(( \nabla \Sigma) \) is defined as \(( \nabla, \Sigma ) = \sum_{j=1}^{2} \partial_j \Sigma_{ij} \).

To describe the boundary conditions, we decompose \( \Gamma_{SL} \) (respectively \( \Gamma_{LG} \)) in two parts \( \Gamma_{SL}^M \) and \( \Gamma_{SL}^m \) (respectively \( \Gamma_{LG}^M \) and \( \Gamma_{LG}^m \)). The notation \( M \) (respectively \( m \)) refers to the macroscopic (respectively mesoscopic) boundary.

The boundary conditions on the free surface (liquid-gas) are

\[
\begin{align*}
\tilde{\Sigma}_n &= (-p_{ext} + \sigma_{LG} \kappa) \tilde{n} & \text{in } (0, T) \times \Gamma_{LG}^M \\
\tilde{\Sigma}_n &= (-p_{ext} + \sigma_{LG} \kappa) \tilde{n} + (\nabla \sigma_{LG} . \tilde{r}) \tilde{r} & \text{in } (0, T) \times \Gamma_{LG}^m 
\end{align*}
\]

(3)

where \( \kappa \) is the mean curvature and \( p_{ext} \) is the external pressure.

The liquid-solid contact is described by

\[
\tilde{u} = \tilde{U}_S & \text{ in } (0, T) \times \Gamma_{SL}^M 
\]

(4)

where \( \tilde{U}_S \) is the solid velocity, and

\[
\begin{align*}
\tilde{u} . \tilde{n} &= 0 & \text{in } (0, T) \times \Gamma_{SL}^m \\
\Sigma_r &= -\beta (\tilde{u} - \tilde{U}_S) - \frac{1}{2} (\nabla \sigma_{SL}) . \tilde{r} & \text{in } (0, T) \times \Gamma_{SL}^m
\end{align*}
\]

(5)

where \( \beta > 0 \) is a sliding type coefficient. We have \( \beta \approx \frac{h}{h} \) where \( h \) is the layer thickness, see [14].

The boundary condition (5) removes the shear-stress singularity. Surface tension gradients appear in (3) and (5). It is one of the particularity of the present model. Let us recall that surface tension gradients imply a flow towards the region of higher surface tension (the Marangoni effect).
The free surface dynamic. We can define the free surface $\Gamma_{LG}$ as the graph of a function $\varphi(t, x_1)$—at least locally—as follows:

$$\Gamma_{LG} = \{ x_2, x_2 = \varphi(t, x_1), x_1 \in I_x, t \in (0, T) \}$$  \hspace{1cm} (6)

Then, the free surface motion is described by transport equation:

$$\frac{\partial \varphi}{\partial t} + u_1 \frac{\partial \varphi}{\partial x_1} = u_2 \quad \text{in} \ (0, T) \times I_x$$  \hspace{1cm} (7)

with initial conditions given. The boundary conditions is:

$$\varphi(t, \hat{x}) \quad \text{given}$$  \hspace{1cm} (8)

if the extremity point $\hat{x}$ of the surface is an inflow extremity.

Using the representation (6) of $\Gamma_{LG}$, we have the expression of the mean curvature:

$$\kappa(t, x_1) = \frac{\partial}{\partial x_1} \left( \frac{\frac{\partial \varphi}{\partial x_1}}{\sqrt{1 + \left( \frac{\partial \varphi}{\partial x_1} \right)^2}} \right)(t, x_1) \quad \text{in} \ (0, T) \times I_x$$  \hspace{1cm} (9)

Remark 2.1 Let us point out an important feature of the model. The dynamic wetting angle $\theta_d$ is not imposed. It is a response of the model. It can be computed using the relation:

$$\cotan(\theta_d) = -\frac{\partial \varphi}{\partial x_1}(t, P_C) \ \text{in} \ (0, T)$$  \hspace{1cm} (10)

2.2 The mesoscopic Local Surface Model

Briefly, the so-called mesoscopic LSM as it is established in [14] is as follows. The interfaces are described by surface densities $\rho^s$. These surface densities are solution of surface continuity equations. A state equation gives the relation between $\rho^s$ and the surface tension coefficients $\sigma$.

We denote by $\rho_{i}^s$, $i = 1, 2$, the surface density on $\Gamma_{LG}$ ($i = 1$) and on $\Gamma_{SL}$ ($i = 2$). The surface tension is related to the excess density through a linear state equation

$$\sigma_i = \gamma(\rho_0^s - \rho_i^s) \quad i = 1, 2.$$  \hspace{1cm} (11)

where $\gamma$ and $\rho_0^s$ are given constants.

We have the surface continuity equation:

$$\frac{\partial \rho_i^s}{\partial t} + \text{div}(\rho_i^s v_i^s) + \frac{1}{\tau_s}(\rho_i^s - \rho_i^q) = 0 \quad i = 1, 2$$  \hspace{1cm} (12)
where $\tau^*$ is the relaxation time relative to the rolling motion, $v_1^*$ is a mean velocity inside the layer and $\rho_i^{eq}$ is its density at equilibrium, \[14\]: $\sigma_i(\rho_i^{eq}) = \sigma_i^{eq}$, $i = 1, 2$.

The velocity $v_1^*$ (respectively $v_2^*$) is related to $\rho_1^*$ (respectively $\rho_2^*$) and to the fluid velocity $u$ (respectively the solid velocity $U_S$). We have the following Darcy laws type, \[14\]:

\[
(1 + 4\alpha_1\alpha_2)\nabla \sigma_{LG} = 4\alpha_2(v_1^* - u) \quad \text{and} \quad v_2^* = \alpha_1\nabla \sigma_{SL} + \frac{1}{2}(u + U_S)
\]  \(13\)

where $\alpha_i$, $i = 1, 2$, are given constants characterizing the viscous properties of the interface.

At the triple junction, the surface flux continuity is imposed:

\[
(\rho_1^* v_1^*)e_f = (\rho_2^* v_2^*)e_g
\]  \(14\)

where $e_f$ and $e_g$ are unit vectors normal to the contact line and tangential to the gas-liquid and gas-solid interface respectively. Let us notice that: $\cos(\theta_d) = -e_f.e_g$.

### 3 THE 1D LOCAL SURFACE MODEL

We consider the 1D steady-state LSM. We reformulate the equations by eliminating the variable $v_1^*$. For both case $i = 1$ and 2, we obtain similar equations. They are non linear degenerated. Case $i = 2$ (solid-liquid surface) leads to:

\[
(P) \begin{cases}
- (\rho \rho')' + \delta_1 U \rho' + \delta_2 \rho = f \quad \text{in } [0,1] \\
\rho(0) = \rho_0 \\
- \rho \rho' + \delta_1 U \rho(1) = \phi
\end{cases}
\]

where $\delta_1 = \frac{U^*}{\lambda \rho^*}$, $\delta_2 = \frac{\rho^*}{\lambda \rho^*}$ are dimensionless numbers, $\phi = \delta_1 \rho_1^{eq}(2U(1) - U(0)) \leq 0$, $\phi$ is the flux at the contact point and $f = \delta_2 \rho_0$. Let us notice that if we set $l = \tau^*U^*$, then $\delta_1 = \delta_2 = \frac{\tau^*[U^*]^2}{\lambda \rho^*}$.

#### 3.1 Mathematical analysis

Let us assume

**Assumption 3.1**

i) $\rho_0 > 0$.

ii) $U \in W^{1,\infty}(0,1)$ and $U \leq 0$ in $[0,1]$; $U' \geq 0$ a.e. and $\|U'\|_\infty \leq \frac{\delta_2}{\delta_1}$.

We consider the non linear regularized problem:

\[
(P^\beta) \begin{cases}
- (\beta_z(\rho) \rho')' + \delta_1 U \rho' + \delta_2 \rho = f \quad \text{in } [0,1] \\
\rho(0) = \rho_0 \\
- \beta_z(\rho) \rho' + \delta_1 U \rho(1) = \phi
\end{cases}
\]
where \( \varepsilon > 0 \), \( \beta_\varepsilon \in C^1(\mathbb{R}) \) is Lipschitz, increasing and defined by: \( \beta_\varepsilon(x) = \varepsilon \) if \( x \leq 0 \) and \( \beta_\varepsilon(x) = x \) if \( x \geq 2\varepsilon \).

Using the Leray-Schauder fixed, we prove that under Assumption 3.1, Problem \( (P^\beta) \) has at least one weak solution in \( H^1(0,1) \) and this solution belongs to \( H^2(0,1) \).

Furthermore, let \( \eta \) be a real satisfying: \( \rho_0 \geq \eta > 0 \) and \( \eta \delta U(1) \geq \phi \). For example with \( U(1) < 0 \), we set: \( \eta = \min\{\rho_0, \frac{1}{\delta U(1)}\} \).

Combining the weak maximum principle, see [8], and the previous existence result, we obtain:

**Theorem 3.1** Under Assumption 3.1, Problem \( (P) \) has at least one weak solution \( \rho \) in \( H^1(0,1) \). This solution satisfies \( \rho(x) \geq \eta > 0 \) in \( [0,1] \) and belongs to \( H^2(0,1) \).

Detailed proof is done in [13].

Let us prove

**Theorem 3.2** Under Assumption 3.1, Problem \( (P) \) has an unique solution \( \rho \).

Proof. We denote by \( \rho_1 \) and \( \rho_2 \) two solutions of \( (P) \).

a) First, we prove that \( \rho_1(0) = \rho_2(0) \). Let us suppose that \( \rho_1(0) > \rho_2(0) \). Let \( [0,\xi_0] \) the largest interval such that \( \rho_1(x) > \rho_2(x), \ x \in [0,\xi_0] \).

Let us suppose \( \xi_0 = 1 \). We integrate the first equation of \( (P) \) on \( [0,1] \) with \( \rho_1 \) and \( \rho_2 \). By differentiating we obtain:

\[-\rho_1\rho_1' + \rho_1\rho_2' + \rho_0(\rho_1 - \rho_2) + \delta U(\rho_1 - \rho_2)\frac{d}{dx} \int_0^1 (\delta_2 - \delta_1 U') (\rho_1 - \rho_2) dx = 0 \]

Using the boundary conditions of \( (P) \), we obtain: \( \int_0^1 (\delta_2 - \delta_1 U') (\rho_1 - \rho_2) dx < 0 \), which is impossible.

Therefore \( \xi_0 \in [0,1] \) and \( \rho_1(\xi_0) = \rho_2(\xi_0) \). As previously, we integrate on \( [0,\xi_0] \) and we obtain:

\[-\rho_1(\xi_0)(\rho_1'(\xi_0) - \rho_2'(\xi_0)) + \rho_0(\rho_1'(0) - \rho_2'(0)) + \int_0^1 (\delta_2 - \delta_1 U') (\rho_1 - \rho_2) dx = 0 \]

hence \( (\rho_1 - \rho_2)'(\xi_0) > 0 \). It is impossible. Therefore, \( \rho_1(0) = \rho_2(0) \).

b) Second, we write the first equation of \( (P) \) as a first order differential equation of the form: \( W'(x) = G(W)(x), \ x \in [0,1] \) with \( W = (u, v)^T \) and

\[ G(W)(s) = (v(s), \frac{-1}{u(s)}[-u^2(s) + \delta_1 U(s)v(s) + \delta_2 u(s) - f(s)])^T \]

We consider \( G : C^1([0,1]; \mathbb{R}) \cap \mathcal{F}^+ \times C^0([0,1]; \mathbb{R}) \to C^0([0,1]; \mathbb{R}) \times C^0([0,1]; \mathbb{R}) \) with \( \mathcal{F}^+ = \{u, \ u \in C^0([0,1]; \mathbb{R}), \ u > 0 \in [0,1]\}. \)
Then, we set $W_i = (\rho_i, \mu_i)^T$, $i = 1, 2$. We have $W_i(x) = G(W_i(x))$, $x \in [0, 1]$, and $W(0) = W(2)$. Hence, $(W_1 - W_2)(x) = \int_0^x (G(W_1) - G(W_2))(s) \, ds$.

Since $\rho_i \in C^1([0, 1], \mathbb{R}) \cap \mathcal{F}$ and $G(W_i)$ is of class $C^1$, there exists a constant $k$ such that: $\|G(W_1) - G(W_2)(s)\| \leq k \|W_1 - W_2(s)\|$. Then, it follows from the previous equality that: $\|(W_1 - W_2)(x)\| \leq k \int_0^x \|(W_1 - W_2)(s)\| \, ds$.

Setting $I(x) = \int_0^x \|(W_1 - W_2)(s)\| \, ds$, we obtain: $\frac{d}{dx}(I(x) \exp(-kx)) \leq 0$. Also, $I(0) = 0$, therefore $I(x) \leq 0 \forall x \in [0, 1]$. Then, we conclude that $W_1 = W_2$ in $[0, 1]$.

**Proposition 3.1** Let Assumption 3.1 be satisfied and $U$ be such that $U(0) > 2U(1)$.

i) If $\phi = \delta U(1)\rho_0$ then $\rho \equiv \rho_0$, $\rho$ being the unique solution of (P).

ii) If $\phi < \delta U(1)\rho_0$ then $\rho(x) \geq \rho_0$ and $\rho'(x) \geq 0$ in $[0, 1]$.

iii) If $\phi > \delta U(1)\rho_0$ then $\rho(x) \leq \rho_0$ and $\rho'(x) \leq 0$ in $[0, 1]$.

**Proof.** i) It is straightforward to verify that $\rho \equiv \rho_0$ is solution and the solution is unique.

ii) We have $\phi < \delta U(1)\rho_0$. Since the weak maximum principle holds, we have $\rho \geq \rho_0$ in $[0, 1]$.

Let us prove that $\rho'(x) \geq 0$. If there exists $\xi_0 \in [0, 1]$ such that $\rho'(\xi_0) < 0$, then

$$-(\rho \rho')'(\xi_0) + \delta U(\xi_0) \rho'(\xi_0) = \delta_2(\rho_0 - \rho(\xi_0)) \leq 0$$

hence $-(\rho \rho')'(\xi_0) = -\frac{1}{2}(\rho^2)'(\xi_0) < 0$. We deduce that $(\rho^2)'(\xi) > 0$ in a neighborhood $\mathcal{V}(\xi_0)$. Therefore $\rho$ is increasing in $\mathcal{V}(\xi_0)$ and $\rho'(\xi) \geq 0$ in $\mathcal{V}(\xi_0)$, which is a contradiction with $\rho'(\xi_0) < 0$. Then, we deduce that $\rho'(x) \geq 0$ in $[0, 1]$ hence in $[0, 1]$ since it is continue. iii) We have $\phi > \delta U(1)\rho_0$. Let us prove that $\rho \leq \rho_0$ in $[0, 1]$. To this end, we suppose that $\max_{[0, 1]} \rho(\xi) = \rho(\xi_m) > \rho_0$.

We have $\xi_m \neq 0$ since $\rho(0) = \rho_0$. Let us suppose $\xi_m \in [0, 1]$.

We write the equation in $\xi_m$: $-(\rho \rho')'(\xi_m) + \delta U(\xi_m) \rho'(\xi_m) + \delta_2 \rho(\xi_m) = \delta_2 \rho_0$. Hence, $-\rho \rho''(\xi_m) = \delta_2(\rho_0 - \rho(\xi_m))$ since $\rho'(\xi_m) = 0$. We deduce $-\rho \rho''(\xi_m) < 0$ and $\rho''(\xi_m) > 0$.

It is a contradiction with the definition of $\xi_m$.

Let us suppose $\xi_m = 1$. We have $\rho'(\xi_m) \geq 0$. Using the boundary condition in $x = 1$, we obtain: $\phi \leq \delta U(1)\rho(1)$. In others respects, $\phi > \delta U(1)\rho_0 > \delta U(1)\rho(1)$. It leads to a contradiction. Therefore, $\rho \leq \rho_0$ in $[0, 1]$.

The proof of $\rho' \leq 0$ in $[0, 1]$ is similar to the previous case ii).

We present some extra properties useful for the numerical analysis.

**Lemma 3.1** Let Assumption 3.1 be satisfied and let $\rho$ be the unique solution of (P). We have:

i) $(\rho - \delta U)(x) \geq 0$ in $[0, 1]$.

ii) If $\phi \leq \delta U(1)\rho_0$ then $\rho'(x) \leq \delta_2$ in $[0, 1]$.

iii) If $\phi > \delta U(1)\rho_0$ and $U^2(0) \leq 4\delta_2 \rho_0$ then $\rho''(x) \leq \delta_2$ in $[0, 1]$.
Proof is done in [13].

Now we prove an useful property of monotony:

**Proposition 3.2** Let Assumption 3.1 be satisfied. Let $A$ be the operator defined by: $A : \mathbb{R} \rightarrow H^1(0,1)$; $\phi \mapsto \rho$, where $\rho$ is the unique solution of $(P)$. Then, the operator $A$ is monotone.

Namely, let $\phi_2 < \phi_1 < 0$, let $\rho_1$ and $\rho_2$ be the unique corresponding solutions, then we have: $\rho_2 \geq \rho_1$ in $[0,1]$.

**Proof.** Case 1. We have: $\phi_2 < \delta U(1) \rho_0 \leq \phi_1 < 0$.

In virtue of Proposition 3.1, $\rho_1 \leq \rho_0 \leq \rho_2$ and the property holds.

Case 2. We have: $\delta U(1) \rho_0 < \phi_2 < \phi_1$.

A. Let us prove that $\rho_1(0) \leq \rho_2(0)$.

In virtue of Proposition 3.1, we have $\rho_i(x) \leq \rho_0$ and $\rho'(x) \leq 0$, $i = 1, 2$, in $[0,1]$.

Let us suppose that $\rho_1'(0) > \rho_2'(0)$. Then, there exists $\xi$ such that $\rho_1 > \rho_2$ in $]0, \xi[$. Let $\xi_{\text{max}}$ be the largest value of $\xi$ such that $\rho_1 > \rho_2$ in $]0, \xi[$.

a) Case $\xi_{\text{max}} = 1$.

Following the same idea of proof than in Theorem 3.2, we integrate the first equation of $(P)$ on $[0,1]$ with $\rho_1$ and $\rho_2$, we differentiate the two equations and we obtain:

$$(\phi_1 - \phi_2) + \rho_0(\rho_1'(0) - \rho_2'(0)) + \int_0^1 (\delta U'(\rho_1 - \rho_2))dx = 0$$

which leads to a contradiction. Hence the case $\xi_{\text{max}} = 1$ is impossible.

b) Case $\xi_{\text{max}} \in ]0, 1[$.

We have: $\rho_1(\xi_{\text{max}}) = \rho_2(\xi_{\text{max}}) = \lambda > 0$.

We integrate the first equation of $(P)$ in $]0, \xi_{\text{max}}[$ and we proceed as previously. We obtain:

$$-\lambda[(\rho_1' - \rho_2')(\xi_{\text{max}})] + \rho_0(\rho_1' - \rho_2')(0) + \int_0^{\xi_{\text{max}}} (\delta U'(\rho_1 - \rho_2))dx = 0$$

Then, we deduce: $(\rho_1' - \rho_2')(\xi_{\text{max}}) > 0$. Hence, $(\rho_1 - \rho_2)$ is increasing in a neighborhood of $\xi_{\text{max}}$, which is in contradiction with $(\rho_1 - \rho_2)(\xi_{\text{max}}) = 0$ and $(\rho_1 - \rho_2)(x) > 0$ in $]0, \xi_{\text{max}}[$.

It follows that: $\rho_1'(0) \leq \rho_2'(0)$.

B. Following the proof of Theorem 3.2, we have: $\rho_1'(0) = \rho_2'(0)$ implies $\rho_1 = \rho_2$ in $[0,1]$.

Since $\phi_1$ not equal to $\phi_2$, necessarily, $\rho_1'(0) < \rho_2'(0)$.

Hence, there exists $\tau$ such that $\rho_2 > \rho_1$ in $]0, \tau[$. Let $\tau_{\text{max}}$ be the largest value of $\tau$ such that $\rho_2 > \rho_1$ in $]0, \tau[$.

Let us suppose $\tau_{\text{max}} < 1$. Then, $\rho_1(\tau_{\text{max}}) = \rho_2(\tau_{\text{max}})$ and $\rho_1'(\tau_{\text{max}}) \geq \rho_2'(\tau_{\text{max}})$.

Let us consider the case $\rho_1'(\tau_{\text{max}}) = \rho_2'(\tau_{\text{max}})$. Theorem 3.2 as applied to the interval $[\tau_{\text{max}}, 1]$ gives $\rho_1 = \rho_2$ and $\phi_1 = \phi_2$; which is impossible.
Therefore, \( \rho_1(\tau_{\text{max}}) > \rho_2(\tau_{\text{max}}) \). We follow the same idea of proof than previously. There exists an interval \( \tau_{\text{max}}, \xi \) such that \( \rho_1 > \rho_2 \). Let \( \tau_{\text{max}}, \xi_{\text{max}} \) be the largest interval such that the property holds. We consider separately the two cases \( \xi_{\text{max}} = 1 \) and \( \xi_{\text{max}} < 1 \) and by integrating the first equation of Problem \( (P) \), we conclude to a contradiction. Finally, we obtain that \( \tau_{\text{max}} = 1 \) and \( \rho_2 \geq \rho_1 \) in \([0, 1]\).

Case 3. For this case, we have: \( \phi_2 < \phi_1 < \delta_1 U(1) \rho_0 \).
The proof is similar to case 2. Hence, the result. \( \square \)

3.2 Finite element numerical analysis

We discretize the 1D steady-state LSM using the Lagrange finite element method. The numerical analysis is done using the framework and results for non-linear problems presented in [2].

We set \( \rho = (\theta + \rho_0) \) and \( V_0 = \{ v \in H^1(0, 1), \: v(0) = 0 \} \). The weak formulation of Problem \( (P) \) is written as follows:

\[
(P) \quad \begin{cases}
\text{Find } \theta \in V_0 \text{ such that:} \\
\quad \langle F(\theta), v \rangle = 0 \quad \forall v \in V_0
\end{cases}
\]

where \( \langle \cdot, \cdot \rangle \) denotes the duality product \( V_0^\prime \times V_0 \). The operator \( F(\cdot) \) is of class \( C^1 \) from \( V_0 \) into \( V_0^\prime \).

We discretize \( (P) \) using a \( P_k \) Lagrange finite element method \((k \in \mathbb{N}, \: k \geq 1)\). To this end, we set: \([0, 1] = U_{i=0,\ldots,(N-1)}[x_i, x_{i+1}]\) and \( h = \min_i(x_{i+1} - x_i) \). We define the finite element spaces: \( V_{0h} = \{ t \in C^0([0, 1]) ; \forall i, \: t|_{[x_i, x_{i+1}]} \in P_k ; \: t(0) = 0 \} \). The discrete model is:

\[
(P_h) \quad \begin{cases}
\text{Find } \theta_h \in V_{0h} \text{ such that:} \\
\quad \langle F_h(\theta), v_h \rangle = 0 \quad \forall v_h \in V_{0h}
\end{cases}
\]

In order to apply the results for non-linear problems presented in [2], we study the linearized problem:

\[
\begin{cases}
\text{Given } f \in V_0^\prime, \: \text{find } \kappa \in V_0 \text{ such that:} \\
\quad \langle DF(\theta) \kappa, v \rangle = \langle f, v \rangle \quad \forall v \in V_0
\end{cases}
\]

where \( \theta \) is the unique solution of \( (P) \). We have:

Lemma 3.2 Under Assumption 3.1 and if \( U^2(0) \leq \frac{4 \alpha^2}{\beta^2} \rho_0 \), the operator \( DF(\theta) \) satisfies the following properties:

i) it is an isomorphism from \( V_0 \) into \( V_0^\prime \),

ii) it is Lipschitzian at \( \theta \), that is there exists \( L > 0 \) such that for all \( \kappa \in V_0 \), \( \|DF(\theta) - DF(\kappa)\|_{C(V_0 \times V_0^\prime)} \leq L \|\theta - \kappa\|_1. \)
Proof is done in [13].

\[ \text{Theorem 3.3 Let Assumption 3.1 be satisfied and } U^2(0) \leq \frac{4 \delta}{3 \beta} \rho_0 \text{. There exists two constants } h_0 > 0, \alpha_0 > 0, \text{ and for } h \leq h_0, \text{ there exists an unique solution } \theta_h \text{ to problem } (P_h) \text{ in the closed ball } B(\theta, \alpha_0). \]

Moreover, there exists a constant c independent of h such that:

\[ \|\theta - \theta_h\|_1 \leq c \inf_{v \in V_h} \|v - \theta_h\|_1 \leq ch \|\theta\|_2 \quad (15) \]

Proof. The result follows straightforwardly from the application of ([2], Theorem 7.1.). As a matter of fact, since Theorem 3.1, Theorem 3.2 and Lemma 3.2 hold, since the bilinear form \( \langle DF(\theta) \rangle \) is \( V_0 \)-coercitive, the estimates proved in ([2], Theorem 7.1.) hold with the constant \( \beta_h = 1 \). Then, (15) holds since \( \theta \) belongs to \( H^2(0,1) \).

3.3 1D LSM numerical tests

We compute numerically the solution of the 1D LSM using a finite difference method. The solution is computed as the steady-state of the unsteady system. The time scheme is the Crank-Nicholson scheme and the non-linear term \( (-\rho \dot{\rho}) \) is linearized using the Newton-Raphson method.

We assume that \( \sigma_{LG} = \sigma_{LG}^0 \). It follows that \( v^*_L = u \) on \( \Gamma_{LG} \). Then, the LSM is reduced to a 1D differential equation in an interval of the \( y \)-axis (on \( \Gamma_{m} \)).

The computation of the 1D mesoscopic LSM provides a profile of \( \nabla \sigma_2 \). This term will be in next section considered as the local Marangoni source term in the Navier-Stokes boundary conditions -HFSM-.

We consider an air-water-glass system: \( \sigma_{LG}^0 = 70, \sigma_{SL}^0 = 20 \) and \( \sigma_{SG}^0 = 50 \text{ mN/m} \). We set \( \rho_0 = 1 \).

In the static case, we have: \( \cos(\theta_s) = \frac{\sigma_{LG}^0 - \sigma_{SL}^0}{\sigma_{LG}^0} \approx 0.429 \) hence \( \theta_s \approx 64.6^\circ \). In the dynamic case, the Young equation is supposed to remain valid and the case \( \theta_d > 90^\circ \) corresponds to: \( \sigma_{SG}^0 = 50 < \sigma_{SL} < \sigma_{LG}^0 = 70 \).

We set \( \tau^* = 10^{-3} \text{ s} \) -see [1]- and \( U^* = 5.10^{-2} \text{ m/s} \). Hence, \( l \approx \tau^* U^* = 5.10^{-5} \text{ m} \).

We set \( U_S = -1 = U_{stokes}(0) \) (the no slip boundary condition value for the bulk flow) and \( U(x) = \frac{1}{t}(U_S + U_{stokes}(x)) = \left( \frac{1}{t}x - 1 \right) \).

It remains to set the following two parameters: the product \( \lambda \rho^* \) and \( \rho^*_1 \). For the present computation we set: \( \lambda \rho^* = 10^{-6} \) and \( \rho^*_1 = 1/5 \). We obtain \( \delta = -2.5 \). In others respects, for obvious computational reasons, we set \( t = 10 \tau^* U^* \) and we obtain \( \delta_1 = 25 \)
and \( \delta_2 = 250 \).

Let us notice that the state equation \( \sigma_i = \gamma(\rho_i^s - \rho_i) \), \( i = 1, 2 \), implies that \( \rho_1^{eq} < \rho_2^{eq} = 1 \).

(Recall: the indice \( \delta_2 \) is relative to the solid-liquid interface, \( \sigma_2 = \sigma_{SL} \).

Let us point out that all the assumptions on data presented in the mathematical analysis section are satisfied.

The functions \( \rho, \rho', \sigma_{SL} \) and \( \sigma'_{SL} \) obtained are presented below and in Fig. 3.3.

We obtained: \( \sigma_{SL}(P_C) = 66.8, \sigma'_{SL}(P_C) = 1.01 \times 10^6, \theta_d = 103.9^\circ, \rho(P_C) = 2.51 \times 10^{-4}, \|\rho'\|_\infty = 175.6 \).

![Graphs of \( \rho, \rho', \sigma_{SL}, \sigma'_{SL} \)](image)

**Figure 2**: \( \rho, \rho', \sigma_{SL}, \sigma'_{SL} \) plotted

Let us precise that the surface tension \( \sigma_{SL} \) and its gradient \( \sigma'_{SL} \) are deduced from the values of \( \rho, \rho' \) and using the state equation \( \sigma_i = \gamma(\rho_i^s - \rho_i) \), \( i = 1, 2 \). As a matter of fact, since \( \sigma_{L,G}^{1} = \gamma(\rho_0^s - \rho_1^{eq}) \) and \( \sigma_{SL}^{1} = \gamma(\rho_0^s - \rho^s) \), one can deduce the values of the constants \( \gamma \) and \( \rho_0^s \). Then, using the state equation: \( \sigma_{SL}(y) = \gamma(\rho_0^s - \rho(y)) \), we obtain the value of the surface tension coefficient \( \sigma_{SL} \). Finally, we have: \( \theta_d = \cos^{-1}(\frac{\sigma_{L,G}^{1} - \sigma_{SL}(P_C)}{\sigma_{L,G}^{1}}) \), where \( P_C \) denotes the triple point liquid-solid-gas.

Qualitatively, this numerical result presents a variation of the surface tension \( \sigma_{SL} \) and a computed dynamical wetting angle \( \theta_d \) mechanically admissible. In the vicinity of the triple point \( P_C \), the gradient \( \sigma_{SL} \) is very large (a maximum amplitude of \( 10^6 \)).

The choice of the two parameters values of \( \lambda \rho^s \) and \( \rho_1^{eq} \) is the main uncertainty of the model. The present choice leads to an admissible surface tension \( \sigma_{SL} \). Let us point out
that the monotony property, see Proposition 3.2, is useful to identify a parameter range leading to admissible solutions in a mechanical point of view.

4 THE 2D HYDRODYNAMIC FREE SURFACE MODEL

We consider the 2D Hydrodynamic Free Surface Model (2)-(8) with $\sigma_{LG}$ and $\nabla \sigma_{SL}$ given and $\Gamma_{LG} = \Gamma_{MG}$ (ie we consider surface tension variations only on the solid-liquid surface). Gravitational force $g$ and external pressure $p_{ext}$ are neglected. Source terms are curvature term, the local Marangoni term and plate velocity. The free surface problem is solved using a classical ALE formulation and characteristic methods, see e.g. [11], [12].

After time discretization, the algorithm of resolution considered is schematized in Fig. 3.

![Figure 3: Algorithm of resolution](image)

4.1 ALE formulation

Principles and notations. The principle is to define an equivalent velocity field $\gamma$ in the sense $\tilde{\gamma} \cdot n = \tilde{u} \cdot n$ on $\partial \Omega$, and preserving the best as possible the mesh inside the fluid domain $\Omega$.

At each time step, first we define the deformation field $\gamma$ on the free surface $\Gamma_{LG}$, then we extend it all over the domain by setting $\gamma = \gamma \tilde{R}$. $\tilde{R}$ being fixed, and by solving Laplace equation: $\Delta \gamma = 0$ in $\Omega$, $\gamma = u_n[1 + \left(\frac{\partial \gamma}{\partial x}\right)^2]^{\frac{1}{2}}$ on $\Gamma_{LG}$ and $\gamma = 0$ on $\partial \Omega / \Gamma_{LG}$.

Let $t \mapsto C(x, \tau; t)$ be the characteristics lines associated to the velocity field $\gamma$, we have:

\[
\begin{align*}
\frac{dC}{d\tau}(x^\tau, \tau; t) &= \tilde{\gamma}(C(x^\tau, \tau; t), t) \\
C(x^\tau, \tau; \tau) &= x^\tau
\end{align*}
\]
One can define the ALE space-time $\Omega^* \times [0, T]$ such that the points $(C(x^*, \tau; t), t)$ are fixed in that space. Then, one defines the ALE variables: $u^* = u \circ C$ and $p^* = p \circ C$. In the ALE space, fluid particles have a velocity $(u - \gamma)$ at first order in time $(t - \tau)$. And for $t = \tau$, one has: $\frac{\partial u^*}{\partial t} = \frac{\partial u}{\partial t} - \gamma^* \nabla u^*$, with $\gamma^* = \gamma \circ C$, see e.g. [10], [11], [7].

If we denote by $t \mapsto X(x, \tau; t)$ the lagrangian characteristics lines (ie those associated to the velocity field $\bar{u}$), ALE method consists to define a regular field $\bar{\gamma}$ such that:

$$\Gamma^i_{LG} = C(\Gamma^0_{LG}, l^0; t) = X(\Gamma^0_{LG}, l^0; t).$$

In other respect, we have the ALE Navier-Stokes formulation -in dimensionless form-:

$$\begin{cases}
\text{Re} \frac{\partial u^*}{\partial t} - \text{div}(\Sigma(\bar{u}^*, p^*))_{ij} + \text{Re}((\bar{u}^* - \bar{\gamma}^*) \nabla)u^*_i = g_i & \text{in } (0, T) \times \Omega, 1 \leq i \leq 2 \\
\text{div}(\bar{u}^*) = 0 & \text{in } (0, T) \times \Omega
\end{cases}$$

with the associated boundary conditions. $\text{Re}$ is the Reynolds number $\text{Re} = \frac{\varepsilon U^* l^*}{\mu}$ with $U^*$ and $L^*$ the characteristic velocity and characteristic length respectively.

The solution $(\bar{u}^*, p^*) \circ C$ is an approximaton of $(\hat{u}, \hat{p})$ at first order in time, and curvatures $\kappa^*$ approximates $\kappa$ at first order in time too.

**Implementation.** In a practical point of view, at each time step, in order to compute the transported free surface and mesh, we proceed as follows, see [11].

1. Given $\bar{u}^n$ on $\Gamma^n_{LG}$, see Fig. 3, we transport the free surface $\Gamma^n_{LG}$ following the lagrangian characteristics lines $X(x, \tau; t)$.
2. We identify a posteriori an equivalent deformation field $\bar{\gamma}^n$.
3. We compute the transport of the full domain $\Omega^n$ by $\bar{\gamma}^n$.

Let us detail each step.

**First step: Transport of $\Gamma_{LG}$ by the lagrangian characteristics method.** We compute the new free surface $\Gamma_{LG}^{n+1} = \{x_2, x_2 = \varphi^{n+1}(t, x_1), x_1 \in I_x\}$ by solving (7) using the characteristics method (ie following the lagrangian $X(x, \tau; t)$ characteristics lines).

Let $x_1$ be a $x_1$-coordinate surface node, $x_k = X(x_k, t^{n+1}; t^n)$. By integrating the characteristics differential system we obtain (at first order in time):

$$\varphi(X(x_k, t^{n+1}; t^{n+1}), t^{n+1}) - \varphi(X(x_k, t^{n+1}; t^n), t^n) = \int_{x_0}^{x_k} u_2^n(x, \varphi^n(x)) dx$$

if $u_1^n(x, \varphi^n(x))$ not equals 0, and

$$\varphi(X(x_k, t^{n+1}; t^{n+1}), t^{n+1}) - \varphi(X(x_k, t^{n+1}; t^n), t^n) = u_2^n(x, \varphi^n(x)) \Delta t$$

if not.

The unknow is the characteristic foot $z_0 = X(x_k, t^{n+1}; t^n)$. $z_0$ is computed using an explicit Euler scheme “element-by-element”, see Fig. 4.

In other words, we transport the boundary nodes of $\Gamma_{LG}^n$ by $\bar{u}$ using a characteristic
method. We obtain the new node positions.

Second step: Computation of $\tilde{\gamma}$. Once, we computed the new value of $\varphi$ for each surface nodes (ie $\varphi^{n+1}(x_k)$, $\forall k$), we deduce an equivalent deformation field $\tilde{\gamma}$. To this end, we set $\tilde{R} = (\partial x_2)$, we set $\gamma$ for each node $x_1$-coordinate by:

$$\gamma(x_k) = \frac{1}{\Delta t}[\varphi^{n+1}(x_k) - \varphi^n(x_k)]$$

Then, we extend the deformation field $\tilde{\gamma}$ by solving the Laplace equation detailed above.

Third step: Mesh Transport. Once the ALE Navier-Stokes system is solved, see Fig. 3, we set $\Omega^{n+1} = \Delta t \tilde{\gamma}(\Omega^n)$.

![Diagram of characteristic method element-by-element and computation of $\tilde{\gamma}$](image)

4.2 Navier-Stokes equations with free surface fixed

Let $\Omega^n$ be given and let $t \mapsto \xi(x, \tau; t)$ be the characteristics lines associated to the deformation field $(\tilde{u} - \tilde{\gamma})$. We solve the ALE Navier-Stokes equations time-discretized using backward Euler method:

$$\begin{cases}
-2 \text{div}(D(\bar{u}^n)_{n+1}) + \nabla(\rho^n)_{n+1} + \frac{Re}{\Delta t} [(\bar{u}^n)^n \circ \xi^n] = \frac{Re}{\Delta t} [0, \xi^n] \\
\text{div}((\bar{u}^n)_{n+1}) = 0
\end{cases} \quad \text{in } \Omega^n \quad \text{(17)}$$

with the associated dimensionless boundary conditions (3)-(5), and $D(u) = \frac{1}{2}(\nabla u + \nabla^T u)$. The term $[(\bar{u}^n) \circ \xi^n]$ is approximated by a characteristic method (first order in time). The Stokes type problem is solved by the Hood-Taylor finite element method (second order method). The pressure equation is solved using the augmented Lagrangian method.
and the Uzawa’s algorithm.
Our software Micralef has been developed using the C++ finite element environment
Rheolef\(^1\).

Let us detail the weak formulation. We define: \( W = \{ u, u \in (H^1(\Omega))^2, u \cdot n = 0 \text{ on } \Gamma_{SL}^n \}; \ W_0 = \{ u, u \in W; u = 0 \text{ on } \Gamma_{SL}^M \} \) and \( W_1 = \{ u, u \in W; u = U_S \text{ on } \Gamma_{SL}^M \} \). With usual notations, the weak formulation is:

\[
\begin{cases}
\text{Find } (u^\tau, p^\tau)^{n+1} \in W_1 \times L^2(\Omega)/\mathbb{R} \text{ such that:} \\
2 \int_\Omega D(u^\tau)^{n+1} : D(v) \, dx - \int_\Omega (p^\tau)^{n+1} \text{div}(v) \, dx + \frac{Re}{\Delta T} \int_\Omega (u^\tau)^n \cdot v \, dx + \beta \int_{\Gamma_{SL}^n} (u^\tau)^n v_2 \, ds \\
= \frac{Re}{\Delta T} \int_\Omega (u^\tau)^n \cdot \xi^n \, v \, ds + \frac{1}{C_a} \int_{\Gamma_{LG}} \kappa v \cdot n \, ds + \int_{\Gamma_{SL}^n} g_{\text{dip}} v_2 \, ds \quad \forall v \in W_0 \\
\int_\Omega \text{div}(u^\tau)^{n+1} q \, dx = 0 \quad \forall q \in L^2(\Omega)/\mathbb{R}
\end{cases}
\]

with \( g_{\text{dip}} = (\beta U_S + \frac{1}{2} \nabla \sigma_{SL}) \), and \( C_a \) is the Capillary number \( C_a = \frac{\mu^*}{\sigma_{SL}} \).

Once the ALE solution \((u^\tau, p^\tau)^{n+1}\) computed in \( \Omega^n \), we have to make the change of variable: \((u^\tau, p^\tau) = (u, p) \circ \mathcal{C} \). To this end, we set: \( u^{n+1}|_{\Omega^{n+1}} = (u^\tau)^{n+1}|_{\Omega^n} \).

4.3 The curvature term

The curvature term is: \( I = \int_{\Gamma_{LG}} \kappa \vec{v} \vec{n} \, ds \). Either we discretize \( \kappa \) using expression (9) or we discretize it as follows, see [11].

Let us assume the graph function \( \varphi(x, \cdot) \) regular enough. Let \( A \) and \( B \) be the extrema points of \( \Gamma_{LG} \) and let \([x_1^{(A)}, x_1^{(B)}]\) be discretized by the set -see Fig. 5:-
\{ \( x_1^{(A)} = x_0, \ldots, x_{N+1} = x_1^{(B)} \) \}.

We have: \( \kappa \vec{n} = \frac{d\tau}{ds} \) hence \( I = \left[ \vec{v} \cdot \tau \right]^B_A - \int_A^B \frac{d\vec{v}}{d\tau} \, d\tau \) ds.

For \( \varphi(x, \cdot) \) piecewise linear, we obtain:

\[
I = \vec{v}(x_{N+1})(\vec{\tau}_B - \vec{\tau}_N) + \sum_{i=1}^N \vec{v}(x_i)(\vec{\tau}_i - \vec{\tau}_{i-1}) + \vec{v}(x_0)(\vec{\tau}_0 - \vec{\tau}_A).
\]

5 NUMERICAL RESULTS

Free surface fixed and no curvature term. Influence of the local Marangoni term. We compute the solution of a simplified HFSM: a steady-state Stokes flow with the free surface given and fixed. In addition, the curvature effect are neglected; we set

\(^1\)P. Saramito and N. Roquet, Rheolef C++ finite element environment, http://www-lmc.imag.fr/lmc-cdp/Pierre.Saramito/rheolef
\( \kappa = 0 \).

The goal is to observe numerically the influence of the Marangoni source term \( \sigma'_{\text{SL}} \) on the bulk fluid motion. The geometry \( \Omega \) considered is presented in Fig. 6.

The test model is the following. Given \( \theta, \sigma'_{\text{SL}} \) and \( \Gamma_{\text{LG}} \), find \((u, p)\) satisfying:

\[
\begin{aligned}
\partial_t \Sigma_{i1} + \partial_i \Sigma_{i2} &= 0, \quad i = 1, 2, \text{ and } \text{div}(u) = 0 \quad \text{in} \quad \Omega \\
\Sigma_n &= \Sigma_\tau = 0 \quad \text{on} \quad \Gamma_{\text{LG}} \cup \Gamma_{\text{out}} \\
u &= U_S \quad \text{on} \quad \Gamma^M_{\text{SL}} \\
u.n &= 0 \quad \text{and} \quad \Sigma_\tau = -\beta(u - U_S) + \frac{1}{2} \sigma'_{\text{SL}} \quad \text{on} \quad \Gamma^m_{\text{SL}}
\end{aligned}
\]  

(18)

The only source terms of the model are \( U_S \) and \( \sigma'_{\text{SL}} \). And, for \( \sigma'_{\text{SL}} \equiv 0 \), the unique solution of (18) is \((u, p) = (U_S, 0)\) (the pressure being defined up to a constant).

Therefore, in the numerical experiments presented below, we observe and measure directly the influence of \( \sigma'_{\text{SL}} \) on the fluid motion in the bulk. In other words, we observe the influence of the local Marangoni term on the macroscopic bulk flow.

**Numerical data.** We set \( U_S = (0, -10^{-2})^T \) and \( L = 10^{-5} \) (in I.S. units). We set \( \tau^* = 10^{-3} \) hence \( l \approx \tau^* U^* = 10^{-3} \) and \( \varepsilon \approx \frac{1}{l} \approx 10^{-2} \).

Following the numerical experiments done in previous section -see Fig. 3.3-, we set the slip coefficient \( \beta \approx \frac{\mu}{h_i} \approx \frac{10^{-5} \tau^*}{10^{-5} \varepsilon} = 10^5 \) (\( h_i \) is the layer thickness), and:

\[
\sigma'_{\text{SL}}(y) = \sigma'_{\text{max}} \times \exp\left(\frac{y - y_m}{y_{cp} - y_m} - 1\right) \times \left(\frac{y - y_m}{y_{cp} - y_m}\right) \quad \text{if} \quad y_m \leq y \leq y_{cp}
\]  

(19)

and \( \sigma'_{\text{SL}}(y) = 0 \) if not; where \( \sigma'_{\text{max}} = 10^4 \), \( y_m \) is the middle point of the boundary part \( \Gamma^m_{\text{SL}} \) and \( y_{cp} \) is the contact point \( y \)-coordinate, Fig. 6. Therefore, the present source term \( \sigma'_{\text{SL}}(y) \) behaves qualitatively like those computed previously, see Fig. 3.3.

First, we consider \( \sigma'_{\text{max}} = 10^3 \). We observe a simple flow.

Second, we consider \( \sigma'_{\text{max}} = 5.10^3 \). We observe a more complex flow. The given source term \( g_{\text{slip}} \) changes of sign in the vicinity of \( 7.8 \times 10^{-4} \). The computed \( y \)-coordinate velocity \( u_2 \) changes of sign too, in the same area. Thus, we observe a local recirculation: the Marangoni term induces a recirculation in the vicinity of the contact line, see Fig. 6.
The computations have been performed on few meshes and no particular mesh sensitivity has been noticed.

Moving free surface with curvature term and dynamical angle. We consider the configuration presented in Fig. 7. The plate is fixed: $U_S = 0$. Because of the curvature source term, the free surface and wetting angle are time-dependent. No local slip type boundary term is considered i.e. $\Gamma_{SL} = \Gamma_{SL}^M$. The inertial term is neglected (Stokes equations). Numerical computations are performed until steady-state is reached, Fig. 7.
Moving plate, no-slip boundary conditions and dynamical angle. The plate is moving at speed $U_S = -10^{-2} m/s$. Only the no-slip boundary condition is considered i.e. $\Gamma_{SL} = \Gamma_{SL}^M$. The inertial term is neglected (Stokes equations).

The free surface evolution is shown in Fig. 8. Time evolution of the wetting angle $\theta_d$ is plotted in Fig. 8.

These numerical experiments present the free behavior of the dynamic wetting angle. Nevertheless, one knows that the no-slip boundary condition (adherence) is, in a mechanical point of view, not admissible.

![Figure 8: Adherence. From left to right. Free surface at t=0 s, t=0.4 s, t=0.8 s and wetting angle $\theta_d$ (°C) vs time](image)

Moving free surface with local Marangoni effect and dynamical angle. The plate is moving at speed $U_S = -10^{-2} m/s$. The local slip boundary condition with surface gradient source term is taking into account i.e $\Gamma_{SL} = \Gamma_{SL}^M \cup \Gamma_{SL}^a$. The inertial term is neglected (Stokes equations).

The slip coefficient and the surface tension gradient are the same as previously: $\beta = 10^5$ and $\sigma_{SL}^a$ is defined by (19) with $\sigma_{\max}^a = 10^4$. Initial shape is the same as Fig. 8.

At $t > 0$, a local recirculation similar to Fig. 6 is observed. Also, a time-dependent wetting angle similar to Fig. 8 is observed. Combination of both phenomena lead rapidly to a great mesh distortion. As a matter of fact, with the present parameters, we observe a kind of “thin film” of fluid sticking on the plate. The fluid domain at $t = 0.1$ s is presented in Fig. 9.

Since the local fluid flow, hence the angle dynamics, strongly depend on parameters such that ($\lambda \rho^*$) and $\rho_1^q$, further investigations are required before interpreting free surface shapes obtained.
REFERENCES


