# A New Model of Diphasic Fluids in Thin Films

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**Abstract** In this work, we are interested in the modelling of diphasic fluids flows in thin films. The diphasic aspect is described by a diffuse interface model, the Cahn-Hilliard equation. The specific geometry (thin domain) allows to replace heuristically the usual Navier-Stokes equations by an asymptotic approximation, a modified Reynolds equation (in which the pressure and the velocity are uncoupled), where the viscosity depends on the composition of the mixture. An existence result on the limit system is stated. since the boundary conditions are chosen in order to model the injection phenomenon, previous results on the Cahn-Hilliard equation cannot be applied, and new estimates have to be obtained. Moreover, we present numerical simulations for lubrication applications to improve the understanding of the cavitation phenomenon.

## 1 Introduction

In lubrication applications, the flow of a fluid between two close surfaces in relative motion is described by an asymptotic approximation of the Navier-Stokes equations, the Reynolds equation. This equation is much easier to study, since the pressure and the velocity can be uncoupled. Indeed, the pressure is shown to be independent of the normal direction to the surfaces, this simplification leads to an equation on the

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pressure only, and the velocity can be deduced from the pressure. This approach was introduced by Reynolds, and has been rigorously justified in [2] for the Stokes equation, and generalized afterwards in many works (Navier-Stokes equations [1], unsteady case [3], compressible fluid (for some perfect gases law) [12]..). It is of interest to investigate how this approach can be used for the case of a two fluid flow. A partial answer to this question has been given in [13].

There are two different approaches to describe multi-phase fluids. The most frequent one in the previous works on the subject for lubrication applications is to consider the interface to be sharp. It consists in introducing a variable viscosity $\eta(x,y)$, which is either equal to the viscosity $\eta_1$ of one fluid or the viscosity $\eta_2$ of the other fluid (that is to say that the fluids are supposed to be non-miscible). The behavior of $\eta$ is described by a transport equation. In that case, under an assumption on the interface, the asymptotic equations can be interpreted as a generalized Buckley-Leverett equation coupled with a generalized Reynolds equation [13]. One of the main disadvantages of the method is that the fluid interface is supposed to be the graph of a function, which hinders for example the formation of bubbles. In addition, this kind of models only takes into account hydrodynamical effects between the two phases.

The second class of models describing diphasic flows are the so-called diffuse interface models. These models are not only based on mechanical considerations but also on chemical properties at the interface between the two fluids, which enable an exchange between the two phases. In this paper, we use the Cahn-Hilliard equation, which involves an interaction potential. To this end, we introduce an order parameter $\varphi$, for example the volumic fraction of one phase in the mixture. This kind of model has already been studied for the complete Navier-Stokes equations in [6], [10].

In this paper, we describe the governing equations (in Section 2) for a diphasic fluid in thin flows, and explain how this model is derived from the Navier-Stokes and the Cahn-Hilliard equation. In Section 3, we state an existence result and sketch out its proof. Lastly, in Section 4, the numerical scheme used for simulations of this model is detailed, and some numerical results are given.

## 2 Governing equations

In order to derive the governing equations, we first recall briefly the approach for obtaining the Reynolds equation from the Navier-Stokes equations. Then we introduce the Cahn-Hilliard equation, which models a mixture of fluids. Last, we obtain the full model for two fluids in a thin domain.

## 2.1 Modelling one fluid in a thin domain

For $\varepsilon > 0$, let $\Omega^\varepsilon$ be a thin domain $\Omega^\varepsilon = \left\{(x,y) \in \mathbf{R}^2,\ 0 < x < L,\ 0 < z < \varepsilon h(x)\right\}$, with $h$ a regular mapping from $[0,L]$ to $\mathbf{R}_+^*$ which is supposed to satisfy $0 < h_m \leq h(x) \leq h_M$. The usual Navier-Stokes equations describe an incompressible fluid flow, coupling the velocity $\mathbf{u} = (u,v)$ and the pressure $p$, which depend on the physical parameters of the fluid (the density $\rho$, the viscosity $\eta$), and the external forces $\mathscr{F}$ (for example the gravity term $\rho g$):

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \operatorname{div}\left(\eta D(\mathbf{u})\right) + \nabla p = \mathscr{F}, \qquad \operatorname{div}\mathbf{u} = 0. \tag{1}$$

In lubrication applications, it is important to take the shear effects into account, and the following boundary conditions are used: Dirichlet boundary conditions are imposed on the velocity on $\{z = 0\}$ and $\{z = \varepsilon h(x)\}$:

$$\forall x \in ]0,L[ \quad u(x,0) = s, \qquad u(x,\varepsilon h(x)) = v(x,0) = v(x,\varepsilon h(x)) = 0. \tag{2}$$

It has been showed in [2] that in a thin domain, the conditions on $\mathbf{u}$ on the lateral part of the boundary only occur in the limit problem (i.e. when $\varepsilon \to 0$) by means of the input flow: indeed, any lateral boundary condition corresponding to a given input flow will lead to the same limit problem. Therefore the lateral boundary conditions are not given explicitly, only the input flow $q$ is given:

$$\int_0^{h(0)} \mathbf{u}|_{x=0} \cdot \mathbf{n} = q, \tag{3}$$

where $\mathbf{n}$ is the external normal to $\partial\Omega$.

With the aid of asymptotic expansions, one shows that the Navier-Stokes equations (1) tend formally to the Reynolds equation when $\varepsilon$ tends to zero. It has been proved in [1] that this limit can be justified rigorously. Introducing the rescaled domain

$$\Omega = \left\{(x,y) \in \mathbf{R}^2,\ 0 < x < L,\ 0 < y < h(x)\right\},$$

the following steady-state equation is obtained to the limit $\varepsilon \to 0$:

$$\partial_y\left(\eta\,\partial_y u\right) = \partial_x p, \qquad \partial_y p = 0, \qquad \partial_x u + \partial_y v = 0. \tag{4}$$

The usual procedure to obtain the Reynolds equation is to integrate twice (4) with respect to $y$, and make use of the boundary conditions (2), $u$ can be expressed as a function of $p$. The incompressibility condition enables to obtain an equation on the pressure only, the Reynolds equation:

$$\partial_x\left(\frac{h^3}{12\eta}\partial_x p\right) = s\partial_x\left(\frac{h}{2}\right). \tag{5}$$

The velocity $\mathbf{u}$ is given as a function of $p$:

$$u(x,y) = \frac{y(y-h)}{2\eta}\partial_x p + s\left(1-\frac{y}{h}\right) \qquad \text{and} \qquad v(x,y) = -\int_0^y \partial_x u(x,z)\,dz. \quad (6)$$

The boundary conditions on $p$ are deduced from the ones on $\mathbf{u}$. Indeed, the choice of $q$ corresponds to a Neumann condition on $p$ at $x = 0$: it follows from (6) that

$$q = \int_0^{h(0)} u(0,y)dy = -\partial_x p(0)\frac{h(0)^3}{12\eta} + \frac{sh(0)}{2}.$$

This expression determines $\partial_x p(0)$ as a function of $q$. Moreover, since the pressure $p$ is defined up to a constant, we have to impose another condition. Finally, the boundary conditions on $p$ read:

$$\partial_x p(0) = \frac{12\eta}{h(0)^3}\left(\frac{sh(0)}{2} - q\right), \qquad p(L) = 0. \quad (7)$$

## *2.2 Modelling a mixture in a thin domain*

### 2.2.1 Modelling a mixture and taking the surface tension into account

In order to describe the mixture of two miscible fluids, we introduce an order parameter $\varphi \in [-1,1]$ (corresponding to the volumic fraction of one fluid in the flow). Then all physical parameters are written as functions of $\varphi$. The viscosity $\eta(\varphi)$ of the mixture is given as function of the viscosities of the two fluids $\eta_1$ and $\eta_2$ by:

$$\frac{1}{\eta(\varphi)} = \begin{cases} \dfrac{1+\varphi}{2\eta_1} + \dfrac{1-\varphi}{2\eta_2} & \text{if } \varphi \in [-1,1], \\ 1/\eta_1 & \text{if } \varphi > 1, \\ 1/\eta_2 & \text{if } \varphi < -1, \end{cases} \quad (8)$$

so that $\varphi = 1$ and $\varphi = -1$ correspond to the fluids of viscosity $\eta_1$ and $\eta_2$ respectively.

In a similar way, the density $\rho$ of the mixture can be defined as a function of $\varphi$. However, the nonhomogeneous case $\rho_1 \neq \rho_2$ induces further difficulties (see [8]) due to the loss of the local conservation equation for the density. We do not wish to take these effects into account in this paper. Therefore, we restrict ourselves to the case $\rho_1 = \rho_2$ (as in [6] for example).

In order to describe the evolution of $\varphi$, we introduce the Cahn-Hilliard equation, which is composed of both a transport term, taking the mechanical effects into account, and a diffusive term modelling the chemical effects. The Cahn-Hilliard equation reads in a dimensionless form:

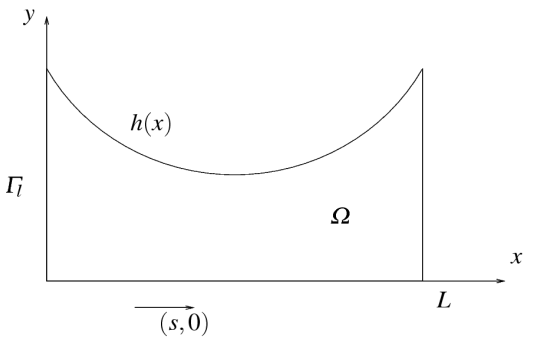


**Fig. 1** Domain $\Omega$ of boundary $\Gamma$ and notations for the boundary conditions on $\varphi$ and on $\mathbf{u}$.

$$\partial_t \varphi + \mathbf{u}\cdot\nabla\varphi - \frac{1}{\mathrm{Pe}}\operatorname{div}(B(\varphi)\nabla\mu) = 0, \tag{9a}$$

$$\mu = -\alpha^2\Delta\varphi + F'(\varphi). \tag{9b}$$

The variable $\mu$ is the chemical potential, $B(\varphi)$ is called mobility, Pe is the Péclet number, $\alpha$ is an non-dimensional parameter measuring the thickness of the diffuse interface, and the function $F$ is called Cahn-Hilliard potential. The physical-relevant assumption on $F$ is that it must have a double-well structure, each of them representing one of the two fluids. A realistic choice for $F$ is given by a logarithmic form $F(x) = 1-x^2+c\,((1+x)\log(1+x)+(1-x)\log(1-x))$, or its polynomial approximation $F(x) = (1-x^2)^2$. The mathematical hypotheses imposed on $F$ match these two choices, and allow some more general profiles. As far as the mobility $B$ is concerned, it is supposed to be regular, positive, and bounded from above and from below: $0 < B_m \le B(\varphi) \le B_M$. Let us mention that other functions $B$ can be considered, in particular the degenerate case $B(x) = (1-x^2)^r$, with $r \ge 0$. This case has been studied in [6], but introduces further mathematical difficulties.

This equation is equipped with boundary conditions on $\varphi$ and $\mu$. Unlike the previous works [6], [10], we are interested in modelling injection phenomena, therefore we consider a Dirichlet condition on $\varphi$ on the left-hand side of the boundary. In order to state the boundary conditions mathematically, we define different parts of the boundary $\Gamma = \partial\Omega$ as follows: let $\Gamma_l = \{(x,y)\in\Gamma, x = 0\}$ be the left-hand part of the boundary (see Fig. 1). Let $\varphi_l$ is a given function satisfying $\varphi_l \in H^{5/2}(\Gamma_l)$, with a compatibility condition reading

$$\exists(\phi_1,\phi_2)\in\mathbf{R}^2, \quad \exists r>0, \qquad \varphi|_{[0,r]} = \phi_1, \quad \varphi|_{[h(0)-r,h(0)]} = \phi_2.$$

The boundary conditions read

$$\varphi|_{\Gamma_l} = \varphi_l, \qquad \frac{\partial\varphi}{\partial\mathbf{n}}\Big|_{\Gamma\setminus\Gamma_l} = 0, \qquad \mu|_{\Gamma_l} = 0, \qquad \frac{\partial\mu}{\partial\mathbf{n}}\Big|_{\Gamma} = 0. \tag{10}$$

In order to take into account the surface tension effects, we add to the external forces $\mathscr{F}$ in (1) an additional term $\kappa\mu\nabla\varphi$, where $\kappa$ is the capillarity coefficient

(related to the surface tension). The Navier-Stokes equation becomes:

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \operatorname{div}\left(\eta D(\mathbf{u})\right) + \nabla p = \kappa\mu\nabla\varphi, \qquad \operatorname{div}\mathbf{u} = 0. \tag{11}$$

The system (11)-(9) has been studied in [6], [10].

### 2.2.2 Modelling diphasic flows in a thin domain

Formally, we can pass to the limit in (11) as $\varepsilon$ tends to zero similarly to Section 2.1. However, it remains to make a choice for the non-dimensionalization of the additional parameters: in this work, $\kappa$ is chosen to be of order $\varepsilon$ (thus the term $\kappa\mu\nabla\varphi$ in (11) vanishes when passing to the limit).

Passing formally to $\varepsilon \to 0$, we get again (4), with $\eta$ non constant. After integrating twice the first equation of (4) and making use of the boundary conditions, we find

$$u = \left(B - \frac{\widetilde{B}}{\widetilde{A}}A\right)\partial_x p + \left(1 - \frac{A}{\widetilde{A}}\right)s \tag{12}$$

where

$$A(x,y) = \int_0^y \frac{dz}{\eta(\varphi(x,z))}, \quad B(x,y) = \int_0^y \frac{z\,dz}{\eta(\varphi(x,z))}, \quad C(x,y) = \int_0^y \frac{z^2 dz}{\eta(\varphi(x,z))}$$

and $\widetilde{A}(x) = A(x,h(x))$, $\widetilde{B}(x) = B(x,h(x))$, $\widetilde{C}(x) = C(x,h(x))$.

As before we use the fact that $\mathbf{u}$ is divergence-free and the boundary conditions to obtain

$$\int_0^{h(x)} \partial_x u(x,z)\,dz = \partial_x \int_0^{h(x)} u(x,z)\,dz = 0.$$

After integrating (12), we have

$$\partial_x\left(\widetilde{D}\partial_x p\right) = s\partial_x\left(\widetilde{E}\right) \tag{13}$$

where

$$\widetilde{D} = \left(\widetilde{C} - \frac{\widetilde{B}^2}{\widetilde{A}}\right) \quad \text{and} \quad \widetilde{E} = \frac{\widetilde{B}}{\widetilde{A}}.$$

The velocity $\mathbf{u} = (u,v)$ is determined from the pressure by:

$$u = \left(B - \frac{A\widetilde{B}}{\widetilde{A}}\right)\partial_x p + \left(1 - \frac{A}{\widetilde{A}}\right)s \qquad \text{and} \qquad v = -\int_0^y \partial_x u(x,z)\,dz. \tag{14}$$

The whole system (Reynolds and Cahn-Hilliard equations) reads, in the case where the capillarity coefficient $\kappa$ is of order $\varepsilon$:

$$\begin{cases} \partial_x(\widetilde{D}(\varphi)\partial_x p) = s\partial_x\widetilde{E}(\varphi) \\ u(x,y) = \left(B - \dfrac{A\widetilde{B}}{\widetilde{A}}\right)\partial_x p + s\left(1 - \dfrac{A}{\widetilde{A}}\right) \\ v(x,y) = -\displaystyle\int_0^y \partial_x u(x,z)dz \\ \partial_t\varphi + u\partial_x\varphi + v\partial_y\varphi - \dfrac{1}{\mathrm{Pe}}\operatorname{div}(B(\varphi)\nabla\mu) = 0 \\ \mu = -\alpha^2\Delta\varphi + F'(\varphi). \end{cases} \tag{15}$$

with the boundary conditions (2), (3), (7), (10), and the initial condition $\varphi|_{t=0} = \varphi_0$, for $\varphi_0 \in H^1(\Omega)$ compatible with the boundary conditions.

*Remark 1.* It is to be noticed that the non-dimensionalization choices for $\alpha$ and $B(\varphi)$ imply that the thin film effect only changes the Reynolds equation, and not the Cahn-Hilliard equation. Other choices lead to different equations, which deserve further studies.

## 3 Theoretical results

Let us state the following existence theorem (the full details of the proof are given in [4]).

**Theorem 1.** *Let us denote* $X(\Omega) = \{f \in H^1(\Omega) \cap L^\infty(\Omega), \partial_y f \in H^1(\Omega)\}$. *Under some smallness assumptions on* $|\Omega|$ *and under a condition on* $F$ *(somehow more general than convexity), there exists a solution* $(p, \mathbf{u}, \varphi, \mu)$ *of* (15)*, equipped with its initial and boundary conditions, such that*

$$\partial_x p \in L^\infty(0,\infty;H^1(0,L)\cap L^\infty(0,L)), \quad u \in L^\infty(0,\infty;X(\Omega)), \quad v \in L^\infty(0,\infty;L^2(\Omega)),$$
$$\varphi \in L^\infty(0,\infty;H^2(\Omega)) \cap L^2_{loc}(0,\infty;H^3(\Omega)), \quad \mu \in L^2_{loc}(0,\infty;H^1(\Omega)).$$

*Proof.* We just sketch out the main steps of the proof, pointing out the main difficulties and differences with previous works [6], [10]. The main idea consists in writing a unique equation on $\varphi$ by expressing $\mathbf{u}$ and $p$ as a function of $\varphi$.

1. Since the Reynolds equation (13) is an elliptic equation on $p$, we have to prove first the regularity of $p$ as a function of $\varphi$, and then deduce the regularity of $\mathbf{u}$ by (14). For the regularity of $p$, the proof divides in two steps; first the proof of the regularity of the coefficients $\widetilde{D}$, $\widetilde{E}$, and then the coercivity of the elliptic operator $\partial_x(\widetilde{D}\partial_x\cdot)$.
2. For the Cahn-Hilliard equation, the usual approach is to use Galerkin approximations, thus reducing the system to finite dimension, and proving the convergence of these approximations.
   We then obtain some a priori estimates on $\varphi$ and $\mu$ in appropriate norms, by multiplying (9a) by $\mu$ and (9b) by $\varphi$ and $\Delta\varphi$, and integrating over $\Omega$:

- The loss of the capillarity term in the limit problem induces difficulties, since usually it cancels with the convection term $\mathbf{u}\cdot\nabla\varphi$ in the Cahn-Hilliard equation. Here, this term of the Cahn-Hilliard equation has to been estimated in order to obtain a priori estimates, and deduce the existence theorem.
- Let us point out that the regularity obtained on the second component $v$ of the velocity is weaker than the regularity obtained with the full Navier-Stokes system ($v \notin L^\infty(\Omega)$). Therefore, the two components of the convection term of the Cahn-Hilliard equation have to be treated separately.
- The boundary conditions on $\varphi$ take into account the fluid injection phenomena, and correspond to a nonhomogeneous Dirichlet condition on the left-hand side of the domain, instead of the homogeneous Neumann condition considered e.g. in [6]. This induces many boundary terms coming from the integration by parts which have to be estimated. It is to be emphasized that the non-conservation of the flow (because of the injection) generates estimates of a slightly different type, which are to be dealt with. Moreover, since the mean value $m(\varphi)$ of $\varphi$ is not constant, classical inequalities on $\varphi - m(\varphi)$ as Poincaré inequality cannot be applied. We have to work with the boundary value of $\varphi$ given on the left-hand side of the domain, and control the terms induced.

3. A Gronwall argument allows to conclude that $\varphi \in L^\infty(0,\infty;H^2(\Omega))$. From the a priori estimates follow weak convergences. For the convergence of the nonlinear term $\mathbf{u}\cdot\nabla\varphi$, we estimate the time derivatives, which allows to conclude the Galerkin process. □

# 4 Numerical simulations

## *4.1 The numerical scheme*

In order to simulate the behavior of a diphasic flow in thin film, we introduce a numerical scheme for the system (15), which consists in two steps. The first step is the computation of the pressure and the velocity by (13) and (14). For the Reynolds equation, the derivatives are discretized by finite differences, and the integrals (in the coefficients) by the trapezoidal method. Then, the Cahn-Hilliard equation is solved using a method similar to the one introduced in [7], [9].

### 4.1.1 Time discretization

For the Cahn-Hilliard equation (9a)-(9b), the time discretization is done with a variable time step $\delta t$. First, knowing the values $\varphi^n$, $\mu^n$ at instant $t^n$, the first step consists in computing the solution $\varphi^{n+1/2}$, $\mu^{n+1/2}$ of the Cahn-Hilliard equation without the convection term, using a $\theta$-method. More precisely, we consider the

following scheme

$$\begin{cases} \dfrac{\varphi^{n+1/2}-\varphi^n}{\delta t} - \dfrac{1}{\mathrm{Pe}}\,\mathrm{div}\left(B(\varphi^n)\nabla(\theta\,\mu^{n+1/2}+(1-\theta)\mu^n)\right) = 0, \\ \theta\,\mu^{n+1/2}+(1-\theta)\mu^n+\alpha^2\Delta(\theta\,\varphi^{n+1/2}+(1-\theta)\varphi^n) = F'(\theta\,\varphi^{n+1/2}+(1-\theta)\varphi^n). \end{cases}$$

The parameter $\theta$ is chosen greater than 0.5 in order to ensure the stability, but close enough to 0.5 so that the precision remains good (for example $\theta = 0.6$). This non-linear system is solved with a fixed point method. From a practical point of view, a few iterations are needed for the method to converge.

For the convection part, knowing $\varphi^{n+1/2}$, we compute $\varphi^{n+1}$ (and then we deduce $\mu^{n+1}$ from $\varphi^{n+1}$ by (9b)). To this end, we define the convection operator $K$ by $K(f) = \mathbf{u}\cdot\nabla f$. The third-order Runge-Kutta scheme reads

$$\varphi^{n+1}-\varphi^{n+1/2} = -\delta t K(\varphi^{n+1/2}) + \frac{1}{2}\delta t^2 K^2(\varphi^{n+1/2}) - \frac{1}{6}\delta t^3 K^3(\varphi^{n+1/2}).$$

#### 4.1.2 Space discretization

The domain considered here is not rectangular, but since there is no particular point where the mesh should be finer, we consider a regular rectangular mesh of uniform cells, and we re-write all the equations in a rescaled rectangular domain.

For a cell $(i,j)$, the values of $p$, $\varphi$ and $\mu$ are sought at the center of the cells (of coordinates $(i,j)$), the values of $u$ at the point of coordinates $(i+1/2,j)$ and the values of $v$ at $(i,j+1/2)$. The boundary conditions are discretized in an usual way, introducing artificial unknowns around the physical domain.

We define a finite-difference centered discretization of the convection operator $K$. In order to ensure that this discretization is $L^\infty$-stable, we use some limiters in the discretization, as proposed for example in [11], and then applied to the Cahn-Hilliard equation in [9]. For this scheme, the C.F.L. (Courant-Friedrich-Levy) condition reads

$$\frac{\delta t}{\delta x}\max_{i,j}(|u_{i+1/2,j}|+|u_{i-1/2,j}|) + \frac{\delta t}{\delta y}\max_{i,j}(|u_{i,j+1/2}|+|u_{i,j-1/2}|) \le 1.$$

### *4.2 The numerical results*

In the field of lubrication, it is of interest to compare the results obtained with the Cahn-Hilliard model with previous results using the Buckley-Leverett equation, for example in [5]. Therefore, we choose the two viscosities of the two fluids to be of ratio $\eta_1/\eta_2 = 10^{-3}$ (which corresponds to the modelling of a lubricant of viscosity $\eta_2$ and air). We simulate a flow between two surfaces in relative motion (i.e. with shear effects). The lubricant is supposed to be adhering to the moving surface, and

the geometry chosen corresponds to a convergent-divergent upper surface: $L = 1$, $h(x) = \frac{1}{3}\left(2(2x-1)^2+1\right)$. In order to work in a rectangular domain, the equations are rescaled. The mesh grid has 1000 elements, and we choose the following numerical data: for the shear velocity $s = 1$, for the input flow $q = 0.28$. The injection height is chosen equal to 0.45 (i.e. for $y \in [0, 0.45]$, lubricant is injected, and for $y \in [0.45, 1]$, air is injected). As for the time evolution, the first simulations are similar to the ones obtained in [5], until a saturation point appears. Then the behavior of the two fluids is significantly different, and we present the numerical simulations in Fig. 2 (the black region corresponds to $\varphi = -1$, i.e. the fluid of viscosity $\eta_2$, the lubricant).

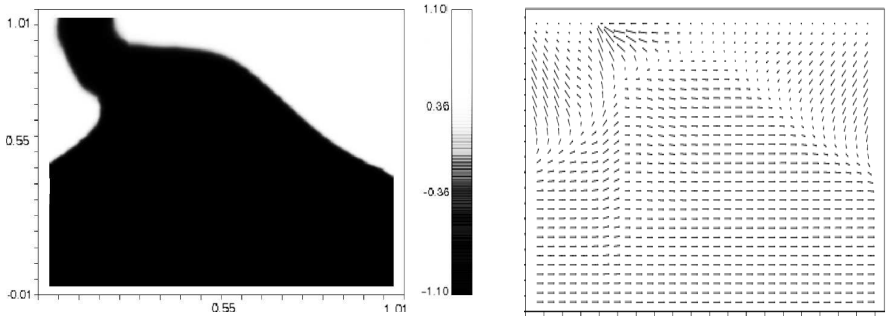


**Fig. 2** Saturation profile (repartition of the two fluids) and velocity field in the thin rescaled domain with convergent-divergent upper surface.

The velocity field obtained in this simulation is similar to the one obtained in previous works. Let us stretch out that the velocity reverses at the left-hand side of the saturation zone. In our model, there is no hypothesis forcing the boundary between the lubricant and air to be the graph of a function. Therefore, on the contrary to [5], the fluid is not limited by a fictive vertical boundary at the left-hand side of the saturation zone, and the saturation profile is consistent with the velocity field.

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