A Kinematic Evolution Equation for the Dynamic Contact Angle and some Consequences

Mathis Fricke\textsuperscript{1}, Matthias Köhne\textsuperscript{2}, and Dieter Bothe\textsuperscript{1,3}

\textsuperscript{1}Department of Mathematics, TU Darmstadt
\textsuperscript{2}Department of Mathematics, HHU Düsseldorf
\textsuperscript{3}Profile Area Thermo-Fluids & Interfaces, TU Darmstadt

Abstract

We investigate the moving contact line problem for two-phase incompressible flows with a kinematic approach. The key idea is to derive an evolution equation for the contact angle in terms of the transporting velocity field. It turns out that the resulting equation has a simple structure and expresses the time derivative of the contact angle in terms of the velocity gradient at the solid wall. Together with the additionally imposed boundary conditions for the velocity, it yields a more specific form of the contact angle evolution. Thus, the kinematic evolution equation is a tool to analyze the evolution of the contact angle. Since the transporting velocity field is required only on the moving interface, the kinematic evolution equation also applies when the interface moves with its own velocity independent of the fluid velocity.

We apply the developed tool to a class of moving contact line models which employ the Navier slip boundary condition. We derive an explicit form of the contact angle evolution for sufficiently regular solutions, which turns out to be unphysical. In particular, it is shown for the simplest model that the contact angle can only relax to equilibrium if a singularity is present at the contact line. We briefly discuss how this inconsistency may be resolved by more general models.

Keywords: Dynamic Contact Line, Kinematics, Navier Slip, Moving Contact Line Singularity

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1 Introduction

We are interested in the evolution of a contact line on a flat and homogeneous solid surface. For this purpose, we consider a two-phase system consisting of two immiscible Newtonian fluids described by the Navier-Stokes equations, in the case where the fluid-fluid interface \( \Sigma \) has contact with a solid. Employing the sharp interface modeling approach, we describe the interfacial layer as a mathematical surface of zero thickness. However, this surface carries additional physical properties like surface tension. The curve of intersection of the fluid-fluid interface with the solid boundary is called the contact line. If the length scale of the flow is sufficiently small, the physical processes at the contact line can have a significant influence on the macroscopic behavior of the system. A typical example is the rise of liquid in a capillary tube with a diameter comparable to the capillary length. The rise height \( H \) of the liquid in the equilibrium state can be found by means of energy considerations and is strongly dependent on the equilibrium contact angle, i.e., the angle of intersection between the fluid-fluid interface and the solid wall

\[
H = \frac{2\sigma \cos \theta_{eq}}{\rho g R}.
\]

However, the mathematical modeling of the dynamics turned out to be a challenging problem, leading to a lot of scientific debate and a great variety of different models ranging from molecular to continuum mechanical descriptions, using both sharp and diffuse interface models. For a recent survey on the field see, for example, \[6\], \[7\], \[19\], \[36\], \[38\] and references therein. While a description on the molecular level can be expected to be more accurate in capturing the physics at the contact line, it is limited in terms of length and time scales for practical applications in the natural and engineering sciences as well as in industry. Therefore, it is desirable to have a continuum mechanical model with an effective description of the necessary physics which is relevant on smaller length scales. However, it turned out that such a model is not straightforward to find. In 1971, Huh and Scriven \[22\] showed that the usual no-slip condition at solid boundaries is not appropriate for the modeling of moving contact lines (see also \[30\], \[59\]). Depending on the model and the solution concept this means that the no-slip condition either leads to the non-existence of solutions with moving contact line or to an infinite viscous dissipation rate. Since then, many attempts have been made to solve this problem, for instance by means of numerical discretization \[2\] (for an overview over numerical methods see \[11\]) and/or by replacing the boundary conditions in the model. Essentially, some mechanism is introduced which allows for a tangential slip of the interfacial velocity at the solid wall. The most common choice for the boundary condition is the Navier slip condition, already proposed by Navier in the 19th century, which relates the tangential slip to the tangential component of normal stress at the boundary.

It has been shown by means of an asymptotic analysis for the stationary Stokes equations \[35\] that the Navier slip condition makes the viscous dissipation rate finite, while the pressure is still singular at the moving contact line (see also \[53\]). This integrable type of singularity is commonly referred to as a weak singularity. There is no agreement in the scientific literature whether or not this type of singularity is acceptable for the description of dynamic wetting. While some authors view it as a manifestation of small-scale physics in the continuum model, it is ruled out in \[35\] by the criterion that the solution shall “remain within the limits of applicability of the model specified via the assumptions made in its formulation.” It is an interesting question under which circumstances the weak singularity is also removed from the description. In the publications \[31\] and \[19\], Ren and Weinan E formulate the expectation that the weak singularity is removed if, instead of a fixed contact angle, a certain model for the dynamic contact angle is applied. The present work shows that this is not the case. Instead, it is shown that the dynamic behavior for sufficiently regular solutions to the simplest model is unphysical (if the slip length is finite). This result can be seen as an extension of the results from \[35\] for quasi-stationary states.

\[\text{Figure 1: Young diagram and equilibrium contact angle.}\]

\[\text{A typical approach to circumvent the problem numerically is to use something called \textit{numerical slip}. The main observation (see \[32\]) that in many cases an artificial slip is introduced by the discretization itself. Due to this numerical effect, the contact line is able to move even though the no-slip condition is used. However, the numerical slip is typically strongly dependent on the grid size. Moreover, the model which is supposed to describe the physics of dynamic wetting is in this case purely numerical and has no physical justification.}\]
It is known that the static contact angle is described by Young’s equation \[ \sigma \cos \theta_{eq} + \sigma_w = 0, \] (1.2)
where \( \sigma_w := \sigma_1 - \sigma_2 \) is the specific energy of the wetted surface (relative to the “dry surface”). The boundary condition in the dynamic case is frequently motivated by experimental observations. The experimentally measured apparent contact angle, which is always subject to a finite measurement resolution, typically shows a strong correlation to the capillary number \( Ca := \frac{\eta V_T}{\sigma} \), where \( V_T \) denotes the contact line velocity. Motivated by this observation, many models prescribe the contact angle as some function of the capillary number and the equilibrium contact angle, i.e.

\[ \theta = f(\theta_{eq}, Ca). \]

Besides these phenomenological models, there are also more advanced continuum models which introduce additional physics into the mathematical description. An interesting candidate within the considered modeling framework (see Remark 1) is the Interface Formation Model due to Y. Shikhmurzaev, which uses interfacial thermodynamics for the description of the contact line region \[ \Sigma(t) \]. Interestingly, this model is able to describe the influence of the flow field onto the dynamic contact angle (“hydrodynamic assist”). Moreover, the dynamic contact angle is given as an output of the model. Models of this type are of course far more complex from an analytical as well as from a numerical point of view. However, from the perspective of the present work, it seems to be unavoidable to go beyond a simple phenomenological approach to get physically reasonable regular solutions in the framework of the two-phase Navier-Stokes equations.

The present work tries to contribute to the mathematical modeling of moving contact lines by analyzing the mathematical properties of the discussed models, in particular the combination of boundary conditions at the contact line, by means of a kinematic approach. The key idea is to understand how the flow field transports the contact angle. Note that here we consider the most simple case of a flat, perfectly clean solid wall and ideal Newtonian fluids, a situation never met in a real-world experiment. A real surface always has some geometrical and chemical structure leading to additional effects like contact angle hysteresis and pinning. Moreover, it might be interesting to consider more complex liquids and substrates to enhance certain properties for applications. However, it seems meaningful to first learn about the mathematics of the problem in the simplest setting.

**Remark 1 (Modeling framework).** In this paper we discuss possible extensions of the Incompressible Two-Phase Navier-Stokes Problem without Phase Transitions (for the modeling see \cite{23, 37, 17, 29}, i.e.

\[
\rho \frac{Dv}{Dt} - \eta \Delta v + \nabla p = 0 \quad \text{in } \Omega \setminus \Sigma(t),
\]
\[
\nabla \cdot v = 0 \quad \text{in } \Omega \setminus \Sigma(t),
\]
\[
[v] = 0, \quad [p I - S] n_\Sigma = \sigma \kappa n_\Sigma \quad \text{on } \Sigma(t),
\]
\[
v = 0 \quad \text{on } \partial \Omega,
\]
\[
V_\Sigma = \langle v, n_\Sigma \rangle \quad \text{on } \Sigma(t)
\]
to the contact line case. Here \( \kappa = - \text{div}_\Sigma n_\Sigma \) denotes the mean curvature of \( \Sigma \), \( S := \eta (\nabla v + \nabla v^T) \) is the viscous stress tensor and \( \sigma > 0 \) is the (constant) surface tension coefficient. The evolution of the interface is determined by \( \Sigma(t) \), where \( V_\Sigma \) denotes the normal velocity of the surface. In the following, we refer to \( (1.3)-(1.7) \) as the “standard model of two-phase flow”. As noted above, the simplest extension is typically done by replacing \( (1.6) \) and adding a contact angle boundary condition.

**Remark 2 (Motivation).** Consider a bounded domain \( \Omega \) (in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \)) with a smooth boundary \( \partial \Omega \). Define a passively advected interface \( \Sigma(t) \) as the zero contour of some level set function \( \phi \), i.e.

\[ \Sigma(t) = \{ x \in \Omega : \phi(x,t) = 0 \}, \]

where \( \phi \) satisfies the transport equation

\[ \partial_t \phi + v \cdot \nabla \phi = 0, \quad t > 0, \quad x \in \Omega, \]
\[ \phi(0, x) = \phi_0(x), \quad x \in \Omega \]
(1.8)

with a given velocity field \( v \). The initial value problem \( (1.8) \) is well-posed if \( v \) is sufficiently regular and tangential to the boundary \( \partial \Omega \), i.e.

\[ v \cdot n_{\partial \Omega} = 0 \quad \text{on } \partial \Omega, \]

where \( n_{\partial \Omega} \) denotes the unit outer normal to \( \partial \Omega \). This can be shown by the method of characteristics. In particular, there is no boundary condition for \( \phi \), i.e. no contact angle can be prescribed. It is well-known from hyperbolic theory that boundary conditions for \( (1.8) \) only have to be imposed at an inflow-boundary, i.e. at points where

\[ v \cdot n_{\partial \Omega}(t,x) < 0. \]

However, many methods for the simulation of flows with contact lines use a time-explicit discretization of the interface transport equation, i.e.

\[ \frac{\phi^{n+1} - \phi^n}{\Delta t} + v^n \cdot \nabla \phi^n = 0, \]
(1.9)
where \( v^n \) is tangential to the boundary, and impose a “contact angle boundary condition”, i.e. a boundary condition for \( \phi^{n+1} \). But from a mathematical point of view, there is no degree of freedom left allowing to impose such a condition. In fact, the evolution of the contact angle is fully determined by the velocity \( v^n \) at time step \( n \) and it has to be “adjusted” or “corrected” afterwards. This observation clearly underlines the need for further understanding.

Organization of the paper: The remainder of this paper is organized as follows. After introducing some basic notation, we derive an evolution equation for the contact angle in Section 2 which we refer to as the kinematic evolution equation. With the help of this result, the time derivative of the contact angle can be expressed by means of the velocity gradient at the contact line. Section 3 recalls the “standard model for two-phase flow” and its extension to contact lines using the Navier boundary condition. The application of the kinematic evolution equation to this class of models is discussed in Section 4. It turns out that the resulting evolution of the contact angle is unphysical. We, therefore, discuss possible generalizations of these models in Section 5.

Notation and mathematical setting: For simplicity, let us assume for this paper that \( \Omega \) is a half space, such that the outer normal \( n_{\Omega} \) is a constant vector. This is not a real restriction for the theory since we are only interested in local properties, but it simplifies the notation. The results may also be generalized for the case of a curved solid wall. Let us now introduce some necessary notation. The following definition of a \( C^{1,2} \)-family of moving hypersurfaces can also be found in [24], [29] and in a similar form in [20].

**Definition 1.** Let \( I = (a, b) \) be an open interval. A family \( \{ \Sigma(t) \}_{t \in I} \) with \( \Sigma(t) \subset \mathbb{R}^3 \) is called a \( C^{1,2} \)-family of moving hypersurfaces if the following holds.

(i) Each \( \Sigma(t) \) is an orientable \( C^2 \)-hypersurface in \( \mathbb{R}^3 \) with unit normal field denoted as \( n_{\Sigma}(t, \cdot) \).

(ii) The graph of \( \Sigma \), given as

\[
\mathcal{M} := \text{gr} \Sigma = \bigcup_{t \in I} \{ t \} \times \Sigma(t) \subset \mathbb{R} \times \mathbb{R}^3, \tag{1.10}
\]

is a \( C^1 \)-hypersurface in \( \mathbb{R} \times \mathbb{R}^3 \).

(iii) The unit normal field is continuously differentiable on \( \mathcal{M} \), i.e.

\( n_{\Sigma} \in C^1(\mathcal{M}) \).

A family \( \{ \Sigma(t) \}_{t \in I} \) is called a \( C^{1,2} \)-family of moving hypersurfaces with boundary \( \partial \Sigma(t) \) if the following holds.

(i) Each \( \Sigma(t) \) is an orientable \( C^2 \)-hypersurface in \( \mathbb{R}^3 \) with interior \( \Sigma(t) \) and non-empty boundary \( \partial \Sigma(t) \), where the unit normal field is denoted by \( n_{\Sigma}(t, \cdot) \).

(ii) The graph of \( \Sigma \), i.e.

\[
gr \Sigma = \bigcup_{t \in I} \{ t \} \times \Sigma(t) \subset \mathbb{R} \times \mathbb{R}^3,
\]

is a \( C^1 \)-hypersurface with boundary \( \text{gr}(\partial \Sigma) \) in \( \mathbb{R} \times \mathbb{R}^3 \).

(iii) The unit normal field is continuously differentiable on \( \text{gr} \Sigma \), i.e.

\( n_{\Sigma} \in C^1(\text{gr} \Sigma) \).

Note that, being the boundary of a submanifold with boundary, the set \( \text{gr}(\partial \Sigma) \) is itself a submanifold (without boundary).

In the remainder of this paper, we consider the following geometrical situation: Let \( \Omega \subset \mathbb{R}^3 \) be a half space and let the “fluid-fluid interface” \( \{ \Sigma(t) \}_{t \in I} \) be a \( C^{1,2} \)-family of moving hypersurfaces with boundary \( \partial \Sigma \) such that

\[
\Sigma(t) \subset \Omega, \partial \Sigma(t) \subset \partial \Omega \quad \forall t \in I,
\]

i.e. the boundary of \( \Sigma \) is contained in the domain boundary. The moving fluid-fluid interface decomposes \( \Omega \) into two bulk-phases, i.e.

\[
\Omega = \Omega^+(t) \cup \Omega^-(t) \cup \Sigma(t),
\]

where the unit normal field \( n_{\Sigma} \) is pointing from \( \Omega^-(t) \) to \( \Omega^+(t) \). The contact line \( \Gamma(t) \subset \partial \Omega \) is the subset of the solid boundary which is in contact with the interface \( \Sigma(t) \), i.e.

\[
\Gamma(t) := \partial \Sigma(t) = \partial \Omega \cap \overline{\Omega^+}(t) \cap \overline{\Omega^-}(t) \neq \emptyset.
\]

We assume that \( \Gamma(t) \) is non-empty and therefore do not consider the process of formation or disappearance of the contact line as a whole. Given a point \( x \in \Gamma(t) \), the contact angle \( \theta \) is defined by the relation

\[
\cos \theta(t, x) := -\langle n_{\Sigma}, n_{\partial \Omega} \rangle(t, x). \tag{1.11}
\]

Local coordinate system: For simplicity of notation, we choose the reference frame where the wall is at rest. Given a point \( x \in \Gamma(t) \) at the contact line, we set up a local coordinate system to describe the evolution of the system. A possible choice is to use \( n_{\Sigma} \) and \( n_{\partial \Omega} \) together with a third linear independent direction. However, the vectors \( n_{\Sigma} \) and \( n_{\partial \Omega} \) are in general not orthogonal and it is more convenient to introduce a contact line normal vector.
The expansions of $\mathbf{u}$ are given by

$$
\mathbf{u}(\mathbf{r}, t) = \mathbf{u}^0(\mathbf{r}) + \mathbf{u}^1(\mathbf{r}, t)
$$

where $\mathbf{u}^0(\mathbf{r})$ is the initial condition and $\mathbf{u}^1(\mathbf{r}, t)$ is the timedependent part.

### 2.5 Boundary Conditions

The boundary conditions are fundamental in ensuring the uniqueness and existence of solutions. They typically involve constraints on the solution or its derivatives at the boundary of the domain.

$$
\mathbf{u}(\mathbf{x}, t) = \mathbf{g}(\mathbf{x}, t), \quad \mathbf{u}(\mathbf{x}, t) = \mathbf{n}(\mathbf{x}, t)
$$

### 2.6 Numerical Methods

Numerical methods are used to approximate the solutions of PDEs when analytical solutions are not available. Common methods include finite difference, finite element, and spectral methods.

$$
\frac{\partial \mathbf{u}}{\partial t} = \mathbf{A}(\mathbf{u}, \mathbf{x}, t), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x})
$$

### 2.7 Applications

The methods and theories discussed in this section are applicable in various fields such as fluid dynamics, heat transfer, and structural mechanics. They provide a framework for modeling and simulating complex physical phenomena.
defined on the interface itself, hence trajectories need to fulfill the time-dependent constraint \( x(t) \in \Sigma(t) \) on \( I \), or, equivalently, \((t, x(t)) \in \text{gr} \Sigma \) on \( I \). A key definition for the theory is the following:

Let \( X \) be a Banach space and \( K \subset X \) a closed subset. Then for \( y \in K \) the Bouligand contingent cone is the set\(^5\)

\[ T_K(y) := \{ z \in X : \liminf_{h \to 0^+} \frac{1}{h} \text{ dist}(y + hz, K) = 0 \}. \]  

(2.1)

An element of \( T_K(y) \) is said to be subtangential to \( K \) at \( y \). If \( K \) is a \( C^3 \)-submanifold the contingent cone coincides with the tangent space of the submanifold. For a boundary point of a submanifold with boundary, it provides a proper generalization. Note that if \( K \subseteq \text{gr} \Sigma \) is a closed subset of \( \text{gr} \Sigma \), then

\[ \text{dist}(y, K) \leq \text{dist}(y, \text{gr} \Sigma) \]  

(2.2)

for all \( y \in K \).

The following result is a special case of Theorem 4.2 in \([13]\) and states that a subtangential and Lipschitz continuous map induces a local semiflow on \( K \). If, in addition, we have that both \( f(y) \) and \( -f(y) \) are subtangential, we obtain a local flow on \( K \) (in forward and backward direction).

In the following, \( B_r^d(x) := \{ y \in \mathbb{R}^d : \| y - x \| < r \} \) denotes the open ball in \( \mathbb{R}^d \) with radius \( r \).

**Theorem 1.** Let \( X = \mathbb{R}^d \), \( K \subset X \) be closed, \( y_0 \in K \), \( K_r := K \cap B_r^d(y_0) \) and \( f : K_r \to X \) be Lipschitz continuous with \( |f(y)| \leq c \) and

\[ f(y) \in T_K(y) \quad \forall \ y \in K_r. \]  

(2.3)

Then the initial value problem

\[ y'(s) = f(y(s)), \quad y(0) = y_0 \]

has a unique solution on \([0, r/c]\) with values in \( K_r \).

**Trajectories on the moving hypersurface:** Given a \( C^{1,2} \)-family of moving hypersurfaces with boundary, we consider a consistent velocity field \( v_\Sigma \in C^1(\text{gr} \Sigma; \mathbb{R}^d) \) satisfying

\[ v_\Sigma : n_\Sigma = V_\Sigma \quad \text{on } \text{gr} \Sigma, \]

\[ v_\Sigma : n_\Gamma = V_\Gamma \quad \text{on } \text{gr} \Gamma. \]  

(2.4)

It follows from (2.3) together with (1.16) that

\[ v_\Sigma(t, x) = V_\Sigma n_\Sigma(t, x) + P_{\Sigma(t)} v_\Sigma(t, x) \]  

(2.5)

\[ \text{if } (t, x) \in \text{gr} \Sigma \text{ and, similarly,} \]

\[ v_\Sigma(t, x) = V_\Gamma n_\Gamma(t, x) + (v_\Sigma, 1t) t(t, x) \]  

(2.6)

\[ \text{if } (t, x) \in \text{gr} \Gamma. \]

Hence, the field \( f \in C^1(\text{gr} \Sigma; \mathbb{R}^d) \) defined by

\[ f(t, x) := (1, v_\Sigma(t, x)) \]

is an element of the tangent space of \( T_{\text{gr} \Sigma}(t, x) \) or \( T_{\text{gr} \Gamma}(t, x) \), respectively (cf. Lemma 1). In order to apply Theorem 1 we set \( X := \mathbb{R} \times \mathbb{R}^3 \), fix a point \((t_0, x_0) \in \text{gr} \Sigma \) and consider the closed subsets

\[ K^d(\Sigma) := \bigcup_{t \in [t_0 - \delta, t_0 + \delta]} \{ t \} \times \Sigma(t) \subset \text{gr} \Sigma, \]

\[ K^d(\Sigma) := K^d(\Sigma) \cap B_r^d(t_0, x_0), \]

\[ K^d(\Gamma) := \bigcup_{t \in [t_0 - \delta, t_0 + \delta]} \{ t \} \times \Gamma(t) \subset K^d(\Sigma), \]

\[ K^d(\Gamma) := K^d(\Gamma) \cap B_r^d(t_0, x_0) \]

for \( \delta > 0 \) sufficiently small.

**Lemma 2.** Under the above assumptions there is \( r > 0 \) such that

\[ \pm(1, v_\Sigma(t, x)) \in T_{K^d(\Sigma)}(t, x) \quad \forall (t, x) \in K^d(\Sigma) \cap \Sigma. \]

Since \( T_{K^d(\Gamma)} \subset T_{K^d(\Sigma)}(t, x) \), it also holds that

\[ \pm(1, v_\Sigma(t, x)) \in T_{K^d(\Sigma)}(t, x) \]  

(2.7)

for all \((t, x) \in K^d(\Sigma)\).

**Proof.** We choose \( r > 0 \) such that \( K^d(\Sigma) \subseteq K^{d/2}(\Sigma) \subseteq K^d(\Sigma) \). Therefore, we do not have to consider the boundary cases \( t = t_0 \pm \delta \).

Let \((t, x) \in K^d(\Sigma) \cap \text{gr} \Sigma \). In this case, the vector \((1, v_\Sigma(t, x))\) is an element of the tangent space of the manifold \text{gr} \Sigma. This follows from (2.5) and Lemma 1. By definition this means that there is an open interval \( I \ni 0 \) and a \( C^1 \)-curve \( \gamma : I \to \text{gr} \Sigma \) such that

\[ \gamma(0) = (t, x), \quad \gamma'(0) = (1, v_\Sigma(t, x)). \]

Clearly, by restriction to a smaller open interval, one can always achieve \( \gamma \in C^1(I; K^d(\Sigma)) \). Therefore, we have

\[ \text{dist}(t, x) + s(1, v_\Sigma(t, x), K^d(\Sigma))] \]

\[ \leq |(t, x) + s(1, v_\Sigma(t, x)) - \gamma(s)| \]

\[ \leq |(t, x) + s(1, v_\Sigma(t, x)) - \gamma(0) - \gamma'(0)s + o(|s|)| \]

\[ = |o(|s|)| \text{ as } s \to 0. \]
Note that this also means that
\[
\text{dist}([t, x] - s(1, v_\Sigma(t, x)), K^4(\Sigma)) = |o([s])|
\]
as \(s \to 0\). Hence it follows that \(\pm (1, v_\Sigma) \in T_{K^4(\Sigma)}\).

Let \((t, x) \in K_0^4(\Gamma) = K_0^4(\Sigma) \cap \text{gr } \Gamma\). Since \((1, v_\Sigma(t, x))\) is an element of the tangent space of the manifold \(\text{gr } \Gamma\), there is an open interval \(I \ni 0\) and a \(C^1\)-curve \(\gamma : I \to K^4(\Gamma)\) such that
\[
\gamma(0) = (t, x), \quad \gamma'(0) = (1, v_\Sigma(t, x)).
\]

With the same argument as above, we obtain
\[
\text{dist}([t, x] \pm s(1, v_\Sigma(t, x)), K^4(\Sigma)) = |o([s])|
\]
as \(s \to 0\).

As a consequence of \eqref{2.7}, Theorem \ref{thm:initial} implies that the initial value problem
\[
\frac{d}{dt} \Phi(t; t_0, x_0) = (1, v_\Sigma(\Phi(t; t_0, x_0))), \quad \Phi(t_0; t_0, x_0) = (t_0, x_0),
\]
is locally uniquely solvable. Since we assume \(v_\Sigma \in C^1(\text{gr } \Sigma)\), standard arguments show that the solution of \eqref{2.8} depends continuously on the initial data \((t_0, x_0)\).

We call the solution \(\Phi(t; t_0, x_0)\) a trajectory on the moving hypersurface. Note that due to the structure of \(\text{gr } \Sigma\), any solution can be written in the form
\[
\Phi(t; t_0, x_0) = (t, \Phi_x(t; t_0, x_0))
\]
with \(\Phi_x(t; t_0, x_0) \in \Sigma(t)\). Since we have that
\[
\pm (1, v_\Sigma(t, x)) \in T_{K^4(\Gamma)} \quad \forall (t, x) \in K^4(\Gamma),
\]
Theorem \ref{thm:initial} also implies that the boundary \(\text{gr } \Gamma\) is an invariant subset, i.e., any trajectory starting in the subset \(\text{gr } \Gamma\) stays in this subset (in both forward and backward direction). Since \(\Phi\) is a flow on \(\text{gr } \Sigma\), it follows that also the interior \(\text{gr } \Sigma\) is an invariant subset (see \cite{2}).

Given these trajectories, the Lagrangian time-derivative of a quantity \(\psi \in C^1(\text{gr } \Sigma)\) is defined as
\[
\frac{D^\Sigma \psi}{Dt}(t_0, x_0) := \frac{d}{dt} \psi(\Phi(t; t_0, x_0)) \bigg|_{t=t_0}.
\]
For an inner point \((t_0, x_0) \in \text{gr } \Sigma\), one may consider the choice
\[
v_\Sigma := V_\Sigma n_\Sigma
\]
and write \(\partial^\Sigma T\) for the corresponding Lagrangian derivative (also called Thomas derivative).

**Theorem 2** (Evolution of the normal vector). Consider a \(C^{1,2}\)-family of moving hypersurfaces and a consistent velocity field \(v_\Sigma \in C^1(\text{gr } \Sigma)\) with
\[
V_\Sigma = \langle v_\Sigma, n_\Sigma \rangle \text{ on } \text{gr } \Sigma.
\]
Then the evolution of the interface normal vector on \(\text{gr } \Sigma\) obeys the evolution equation
\[
\frac{D^\Sigma n_\Sigma}{Dt} = -\sum_{k=1}^2 \langle \partial_{\xi_k} v_\Sigma, n_\Sigma \rangle \tau_k,
\]
where \(\{\tau_1, \tau_2\}\) is an orthonormal basis of \(T_{\Sigma(t_0)}(x_0)\).

**Remark 3.** Since \(V_\Sigma(t, \cdot) = \langle v_\Sigma(t, \cdot), n_\Sigma(t, \cdot) \rangle \in C^1(\Sigma(t))\), equation \eqref{3.2} can be written as
\[
\frac{D^\Sigma n_\Sigma}{Dt} = \sum_{k=1}^2 \langle \partial_{\xi_k} v_\Sigma, n_\Sigma \rangle \tau_k.
\]
In particular, for \(v_\Sigma(t, x) := V_\Sigma(t, x) n_\Sigma(t, x)\) we obtain (in agreement with \cite{24}, Theorem 5.15)
\[
\partial^\Sigma n_\Sigma = -\nabla^\Sigma V_\Sigma.
\]
With this notation, we may express \eqref{2.12} as
\[
\partial^\Sigma n_\Sigma = \partial^\Sigma V_\Sigma + \langle \nabla^\Sigma n_\Sigma, \langle v_\Sigma \rangle \rangle \partial_{\xi_a} n_\Sigma,
\]
where \(w := \langle v_\Sigma \rangle \parallel \langle v_\Sigma \rangle \parallel (\parallel v_\Sigma \parallel)\).

**Theorem 3** (Evolution of the contact angle). Consider a \(C^{1,2}\)-family of moving hypersurfaces with boundary and a consistent velocity field \(v_\Sigma \in C^1(\text{gr } \Sigma)\) with
\[
V_\Sigma = \langle v_\Sigma, n_\Sigma \rangle \text{ on } \text{gr } \Sigma,
\]
\[
V_\Gamma = \langle v_\Sigma, n_\Gamma \rangle \text{ on } \text{gr } \Gamma.
\]
Let \(\Omega\) be a half-space such that \(n_\Omega = 0\) is constant along the boundary and let \(\theta \in (0, \pi)\). Then the time derivative of the contact angle on \(\text{gr } \Gamma\) obeys the evolution equation
\[
\frac{D^\Sigma \theta}{Dt} = \langle \partial_{\xi_a} v_\Sigma, n_\Sigma \rangle, \quad \text{for } \theta = -\cos \theta n_\Gamma - \sin \theta n_\Omega.
\]

**Remark 4.** (i) There is a short way to (formally) derive the kinematic evolution equation \eqref{3.2} using the level set formulation. For details see \cite{18}.
The inverse function has the form
\[
D^\Sigma \theta \frac{\partial}{\partial t} = \partial_{x} V_{\Sigma} + \cos \theta V_{T} (\tau, \partial_{x} n_{\Sigma}) - (v_{\Sigma}, V_{T}) (t, \partial_{x} n_{\Sigma}).
\]
In particular, for the two-dimensional case we obtain
\[
D^\Sigma \theta \frac{\partial}{\partial t} = \partial_{x} V_{\Sigma} - \kappa \cos \theta V_{T}.
\]
In a frame of reference, where the contact line is at rest (i.e. \( V_{T} = 0 \)), the latter formula reduces to
\[
D^\Sigma \theta \frac{\partial}{\partial t} = \partial_{x} V_{\Sigma}.
\]
(iii) Note that for \( \theta \to 0 \) or \( \theta \to \pi \), the interface tangent vector \( \tau \) becomes tangential to \( \partial \Omega \) and \( n_{\Sigma} \to \pm n_{\Omega} \). Therefore, we obtain in the limit
\[
D^\Sigma \theta \frac{\partial}{\partial t} \bigg|_{\theta=0} = D^\Sigma \theta \frac{\partial}{\partial t} \bigg|_{\theta=\pi} = 0.
\]
In the following, we restrict ourselves to the case of partial wetting, i.e.
\[
0 < \theta < \pi.
\]

Preliminaries for the proof: In order to prove Theorem 2 we need a continuously differentiable dependence of the trajectories \( \Phi(\cdot, t_{0}, x_{0}) \) on the initial position \( x_{0} \in \Sigma(t_{0}) \). To this end, we construct a \( C^{1} \)-extension of the velocity field \( v_{\Sigma} \) to an open neighborhood of \((t_{0}, x_{0})\) in \( \mathbb{R}^{4} \), which still leaves \( \text{gr} \Sigma \) invariant. This construction allows to obtain the \( C^{1} \)-dependence on the initial position from standard ODE theory. To show the following Lemma, it is helpful to use a special type of local parametrization for \( \text{gr} \Sigma \) which is constructed in the Appendix.

**Lemma 3** (Signed distance function). Let \( \{ \Sigma(t) \}_{t \in \mathbb{I}} \) be a \( C^{1,2} \)-family of moving hypersurfaces and \((t_{0}, x_{0})\) be an inner point of \( \mathcal{M} = \text{gr} \Sigma \). Then there exists an open neighborhood \( U \subset \mathbb{R}^{4} \) of \((t_{0}, x_{0})\) and \( \varepsilon > 0 \) such that the map
\[
X : (\mathcal{M} \cap U) \times (-\varepsilon, \varepsilon) \rightarrow \mathbb{R}^{4},
\]
\[
X(t, x, h) := (t, x + h n_{\Sigma}(t, x))
\]
is a diffeomorphism onto its image \( N^{\varepsilon} := X((\mathcal{M} \cap U) \times (-\varepsilon, \varepsilon)) \subset \mathbb{R}^{4} \), i.e. \( X \) is invertible there and both \( X \) and \( X^{-1} \) are \( C^{1} \). The inverse function has the form
\[
X^{-1}(t, x) = (\pi(t, x), d(t, x))
\]
with \( C^{1} \)-functions \( \pi \) and \( d \) on \( N^{\varepsilon} \).

The set \( N^{\varepsilon} \) is called “tubular neighborhood” for \( \mathcal{M} \) at the point \((t_{0}, x_{0})\). The function \( d \) is the signed distance to \( \mathcal{M} \) and \( \pi \) is the associated projection operator. For a fixed hypersurface \( \Sigma \), this result is well-known (see, e.g., [21], [29]). The above time-dependent result is already stated without details of the proof in [24], Lemma 5.12. For completeness, we include a short proof.

**Proof.** According to Lemma [A.1] (cf. Appendix), we can choose a local \( C^{1} \)-parametrization \( \phi \) of \( \mathcal{M} \) of the form (with \( \delta, \varepsilon > 0 \), \( U_{0} \subset \mathbb{R}^{4} \) open)
\[
\phi : (t_{0} - \delta, t_{0} + \delta) \times B_{\varepsilon}^{2}(0) \rightarrow \mathcal{M} \cap U_{0},
\]
where \( \phi \) has the following form
\[
\phi(t, u) = (t, \hat{\phi}(t, u)), \quad \phi^{-1}(t, x) = (t, u(t, x)).
\]
Then \( X \) can be expressed as
\[
X(t, x, h) = X^{0}(\phi^{-1}(t, x), h)
\]
with
\[
X^{0}(t, u, h) := (t, \hat{\phi}(t, u) + h n_{\Sigma}(t, \hat{\phi}(t, u))).
\]
The function
\[
X^{0} : I_{\delta}(t_{0}) \times B_{\varepsilon}^{2}(0) \times \mathbb{R} \rightarrow \mathbb{R}^{4}
\]
is continuously differentiable (since \( \hat{\phi} \in C^{1}(I_{\delta}(t_{0}) \times B_{\varepsilon}^{2}(0)) \) and \( n_{\Sigma} \in C^{1}(\mathcal{M}) \)) and the Jacobian of \( X^{0} \) has the form
\[
(\text{DX}^{0})(t, u, h) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
* & D X^{0}_{t}(u, h) & * & *
\end{pmatrix},
\]
where \( X^{0}_{t} \) corresponds to \( X^{0} \) at fixed \( t \), i.e.
\[
X^{0}_{t}(u, h) := \hat{\phi}(t, u) + h n_{\Sigma}(t, \hat{\phi}(t, u)).
\]
Obviously, \( \text{DX}^{0} \) is invertible at \((t, u, h)\) if and only if \( \text{DX}^{0}_{t} \) is invertible at \((u, h)\). The invertibility of \( \text{DX}^{0}_{t} \) at the point \((0, 0)\) is a well-known result from the theory of \( C^{2} \)-hypersurfaces. In particular, one can show by the Banach contraction principle that \( \text{DX}^{0}_{t} \) is invertible on \( B_{\varepsilon}^{2}(0) \times (-\varepsilon(t), \varepsilon(t)) \) if (see [29], chapter 2.3 for details)
\[
\varepsilon(t) \| \nabla_{\Sigma} n_{\Sigma}(t, \hat{\phi}(t, \cdot)) \|_{C(B_{\varepsilon}^{2}(0))} < 1.
\]
Since \( n_{\Sigma} \in C^{1}(\mathcal{M}) \), we can choose for every compact subset \( I \subset I_{\delta}(t_{0}) \) an \( \varepsilon > 0 \) such that (2.15) holds for all \( t \in I \) with \( \varepsilon(t) := \varepsilon \). In particular, \( \text{DX}^{0}_{t} \) is invertible at the point \((t_{0}, 0, 0)\). Now it follows from
the Implicit Function Theorem that there are open neighborhoods $V$ of $(t_0,0,0)$ and $U \subseteq U_0$ of $(t_0,x_0) \in \mathbb{R}^4$ such that $X^0 : V \to U$ is a bijection and both $X^0$ and $(X^0)^{-1}$ are $C^1$. Since the parametrization $\phi : I(t_0) \times B^2(0) \to M \cap U_0$ is a diffeomorphism between manifolds, the claim for $X$ follows from the properties of $X^0$.

We now employ Lemma 3 and set

$$v(t, x) := v_{\Sigma}(\pi(t, x))$$

on the tubular neighborhood $N^\varepsilon$ to construct a local $C^1$-continuation of $v_{\Sigma}$. Note that $v$ generates a local flow map $\Phi$ in an open neighborhood of $(t_0, x_0) \in \mathbb{R}^4$ by means of (2.8). The moving hypersurface $gr \Sigma$ is invariant with respect to $\Phi$ because of the consistency conditions $T^\varepsilon$. Hence we drop the tilde notation in the following. It is well-known from classical ODE theory that a $C^1$-right hand side yields a continuously differentiable dependence on the initial data. Therefore, we have the following result.

**Lemma 4 (Regularity of the flow map).** Let $x_0 \in \Sigma(t_0)$ and $v \in C^1(U)$ for an open neighborhood $U$ of $(t_0, x_0) \in \mathbb{R}^4$. Then $\Phi(t; t_0, \cdot)$ is $C^1$ on an open neighborhood of $(t_0, x_0) \in \mathbb{R}^4$.

**Lemma 5 (Tangent transport).** Under the assumptions of Theorem 3 consider an inner point $(t_0, x_0) \in gr \Sigma$ and a normalized tangent vector $\tau \in T_{\Sigma(t_0)}(x_0)$. Choose a curve $\gamma^0((-\delta, \delta); \Sigma(t_0))$ such that

$$\gamma^0(0) = x_0, \quad (\gamma^0)'(0) = \tau.$$

For simplicity let $\| (\gamma^0)' \| = 1$ on $(-\delta, \delta)$. Then the curve is transported by the flow-map according to

$$\gamma(s, t) := \Phi_x(t; t_0, \gamma^0(s)).$$

Likewise, a time evolution for the tangent vector is defined by

$$\tau(t) := \frac{\partial}{\partial s} \gamma(s, t) \bigg|_{s=0}.$$  \hspace{1cm} (2.17)

The vector $\tau(t)$ is tangent to $\Sigma(t)$ at the point $\Phi_x(t; t_0, x_0)$ since $\gamma^0(t, t) \subset \Sigma(t)$. Moreover, its time derivative is given as

$$\tau'(t_0) = \frac{\partial v_{\Sigma}}{\partial \tau(t_0)}(t_0, x_0).$$

**Proof.** By definition, we have

$$\tau'(t_0) = \frac{\partial}{\partial t} \left( \frac{\partial \Phi_x(t; t_0, \gamma^0(s))}{\partial s} \right)_{s=0} |_{t=t_0}. $$

Since $\gamma \in C^1$ and the second partial derivative

$$\frac{\partial}{\partial s} \frac{\partial}{\partial t} \gamma(s, t) = \frac{\partial}{\partial s} \frac{\partial}{\partial t} \Phi_x(t; t_0, \gamma^0(s)) = \frac{\partial}{\partial s} v_{\Sigma}(\tau(t; t_0, \gamma^0(s))) = \nabla_{\Sigma} v_{\Sigma}(\tau(t; t_0, \gamma^0(s))) \cdot \frac{\partial}{\partial s} \Phi_x(t; t_0, \gamma^0(s))$$

is continuous at $(0, t_0)$, it follows from the Theorem of Schwarz that we can interchange the order of differentiation to obtain

$$\tau'(t_0) = \frac{\partial}{\partial s} \left( \frac{\partial \Phi_x(t; t_0, \gamma^0(s))}{\partial t} \right)_{t=t_0} |_{s=0} = \frac{\partial v_{\Sigma}}{\partial \tau(t_0)}(t_0, x_0). \hspace{1cm} \Box$$

**Proof of Theorem 2** We choose two curves $\gamma^0_1, \gamma^0_2 \in C^1((-\delta, \delta); \Sigma(t_0))$ such that

$$\gamma^0_1(0) = x_0, \quad (\gamma^0_1)'(0) = \tau_1, \quad (\gamma^0_2)'(0) = \tau_2$$

with $|\tau_1| = |\tau_2| = 1$ and $v_{\Sigma}(\tau_1(t_0, x_0), \tau_2(t_0, x_0)) = \tau_1 \times \tau_2$. The flow map $\Phi$ defines a time-evolution of $\gamma^0_1$ and of the tangent vectors $\tau_1$ according to (2.16) and (2.17). As long as $\tau_1$ and $\tau_2$ are linearly independent (i.e., $\tau_1 \times \tau_2 \neq 0$), it follows that

$$n_{\Sigma}(\Phi(t; t_0, x_0)) = \frac{\tau_1(t) \times \tau_2(t)}{|\tau_1(t) \times \tau_2(t)|}$$

and in particular

$$\frac{D^\Sigma n_{\Sigma}}{Dt} \bigg|_{t=t_0} = \frac{d}{dt} \left( \frac{\tau_1(t) \times \tau_2(t)}{|\tau_1(t) \times \tau_2(t)|} \right) \bigg|_{t=t_0}. \hspace{1cm} (2.19)$$

Note that the linear independence of $\tau_1(t)$ and $\tau_2(t)$ for $t$ sufficiently close to $t_0$ follows from the initial condition, i.e.

$$|\tau_1(t_0) \times \tau_2(t_0)| = 1,$$

since $\tau_1(t)$ and $\tau_2(t)$ are continuous. From (2.19) it follows that

$$\frac{D^\Sigma n_{\Sigma}}{Dt} = \tau_1'(t_0) \times \tau_2(t_0) + \tau_1(t_0) \times \tau_2'(t_0)$$

$$- \frac{\tau_1(t_0) \times \tau_2(t_0)}{|\tau_1(t_0) \times \tau_2(t_0)|^2} \frac{d}{dt} |\tau_1(t) \times \tau_2(t)|_{t=t_0}.$$
where $P_{\Sigma} := \mathbf{1} - \langle n_{\Sigma}, \cdot \rangle n_{\Sigma}$ denotes the orthogonal projection onto $\Sigma$. Using (2.18) we conclude
\[\frac{D\Sigma}{Dt} n_{\Sigma} = P_{\Sigma}[(\partial_{\tau_{1}} v_{\Sigma}) \times \tau_{2} + \tau_{1} \times (\partial_{\tau_{2}} v_{\Sigma})].\]
The claim follows by expanding $\partial_{\tau_{1}} v_{\Sigma}$ and $\partial_{\tau_{2}} v_{\Sigma}$ in the basis $\{\tau_{1}, \tau_{2}, n_{\Sigma}\}$.

**Proof of Theorem 3** We first show that equation (2.11) also holds at the contact line. As a result, we obtain the evolution of the contact angle.

For $(t_{0}, x_{0}) \in \text{gr} \Gamma$ we choose a sequence of points $(x_{k}^{0})_{k} \subset \Sigma(t_{0})$ such that $x_{k}^{0}$ converges to $x_{0}$ and consider the trajectories $x^{k}(t)$ defined by
\[\frac{d}{dt} x^{k}(t) = v_{\Sigma}(t, x^{k}(t)), \quad x^{k}(t_{0}) = x_{k}^{0}. \quad (2.20)\]
Moreover, we define the limiting trajectory $x(t)$ starting from $x_{0}$ and running on $\text{gr} \Gamma$. Since $\text{gr} \Sigma$ is invariant under the flow, the evolution equation (2.11) holds along $x^{k}$ for every $k$. Since $\Sigma_{k} \in C^{1}(\text{gr} \Sigma)$, one can choose fields $\tau_{1}, \tau_{2} \in C^{1}(\text{gr} \Sigma)$ such that $(\tau_{1}(t, x), \tau_{2}(t, x))$ is an orthonormal basis to the tangent space of $\Sigma(t)$ at the point $x$ such that
\[n_{\Sigma}(t, x) = \tau_{1}(t, x) \times \tau_{2}(t, x) \quad \text{on} \quad \text{gr} \Sigma.\]

Hence we obtain by integration
\[n_{\Sigma}(t, x^{k}(t)) = n_{\Sigma}(t_{0}, x_{0}^{k}) - \sum_{j=1}^{2} \int_{t_{0}}^{t} \frac{1}{\langle \nabla_{\Sigma} v_{\Sigma} \rangle} \tau_{j}(s, x^{k}(s)) ds.\]

It follows from the continuous dependence on the initial data that the trajectories converge pointwise to the limiting trajectory, i.e.
\[\lim_{k \to \infty} x^{k}(t) = x(t) \quad \text{on} \quad \Gamma(t).\]

Now we pass to the limit and obtain
\[n_{\Sigma}(t, x(t)) = n_{\Sigma}(t_{0}, x_{0}) - \sum_{j=1}^{2} \int_{t_{0}}^{t} \frac{1}{\langle \nabla_{\Sigma} v_{\Sigma} \rangle} \tau_{j}(s, x(s)) ds.\]

Differentiation with respect to $t$ proves that (2.11) also holds at the contact line.

It follows from the definition of $\theta$ that
\[\frac{D\Sigma}{Dt} \cos \theta = -\frac{D\Sigma}{Dt} \langle n_{\Sigma}, n_{\partial \Omega} \rangle.\]

Since $n_{\partial \Omega}$ is constant, we obtain
\[-\sin \theta \frac{D\Sigma}{Dt} \theta = -\langle D\Sigma n_{\Sigma}, n_{\partial \Omega} \rangle.\]

We choose
\[\tau_{1} = \tau = -\cos \theta n_{\Gamma} - \sin \theta n_{\partial \Omega}, \quad \tau_{2} = t_{\Gamma}\]
and proceed using equation (2.11) to arrive at
\[\sin \theta \frac{D\Sigma}{Dt} \theta = -\langle \partial_{\tau_{1}} v_{\Sigma}, n_{\partial \Omega} \rangle - \langle \partial_{\tau_{2}} v_{\Sigma}, n_{\partial \Omega} \rangle (t_{\Gamma}, n_{\partial \Omega}) = \sin \theta \langle \partial_{\tau_{1}} v_{\Sigma}, n_{\Sigma} \rangle.\]

This proves the claim since $\theta \in (0, \pi)$.

### 3 Two-phase flow model

We recall the “standard (sharp interface) model for two-phase flow” and its extension to contact lines using the Navier boundary condition. To formulate the model, we need the notion of the jump of a quantity across the interface $\Sigma$.

**Definition 4** (Jump across $\Sigma$). Fixing an interface configuration $\Sigma$, we define the space $\mathcal{J}(\Omega, \Sigma)$ of continuous functions on $\Omega^{\pm}$, admitting continuous extensions to $\overline{\Omega^{\pm}}$, i.e.
\[\mathcal{J}(\Omega, \Sigma) := \{ \psi \in C(\Omega \setminus \Sigma), \ \exists \lim_{\substack{\pm \to 0^+}} \psi \in C(\overline{\Omega^{\pm}}) \text{ s.t. } \psi \big|_{\Omega^{\pm}} = \psi^{\pm} \}.\]

The jump of $\psi$ across the interface $\Sigma$ at $x \in \Sigma$ is defined as
\[\|\psi\|_{x} := \lim_{n \to \infty} (\psi^{+}(x_{n}) - \psi^{-}(y_{n})),\]
where $(x_{n})_{n \in \mathbb{N}} \subset \overline{\Omega^{+}}$ and $(y_{n})_{n \in \mathbb{N}} \subset \overline{\Omega^{-}}$ are sequences with
\[\lim_{n \to \infty} x_{n} = \lim_{n \to \infty} y_{n} = x.\]

By definition of $\mathcal{J}$, the jump of $\psi$ does not depend on the choice of sequences. Note that away from the boundary $\partial \Omega$, the jump of a quantity $\psi$ may equivalently be expressed as
\[\|\psi\|_{x} := \lim_{h \to 0^+} (\psi(x + hn_{\Sigma}) - \psi(x - hn_{\Sigma})).\]

For $\psi \in \mathcal{J}(\Omega, \Sigma)$ it follows directly from the definition that $\|\psi\|$ is a continuous function on $\Sigma$.

In general, the interface is transported with an independent interface velocity $v_{\Sigma}$. However, up to Section 5 we assume that the velocity field $v = v(t, x)$ is continuous, i.e. $\|v\| = 0$, which physically means that there is no phase change and no slip at the interface. In this case, the interface velocity $v_{\Sigma}$ coincides with the fluid velocity $v$. 
Remark 5 (Regularity). In the following, we consider an open interval $I$ and the space of functions
\[ V := C(I \times \Omega) \cap C^1(\partial \Omega) \cap C^1(\partial^\ast \Omega). \] (3.1)

Note that we assume in particular that the fluid velocities $v^\pm$ are differentiable at the contact line and the viscous stress is locally bounded. This is a rather strong assumption in contrast to weak solution concepts which allow an integrable singularity in the viscous stress as long as the corresponding dissipation rate is finite. However, following the analysis [35] for the Stokes problem, the latter leads to a singularity in the pressure at the moving contact line.

3.1 Energy balance

We recall the basic modeling assumptions leading to the “standard model”. It is assumed that the flow in the bulk phases is incompressible and no mass is transferred across the fluid-fluid and the fluid-solid interface. As a further simplification, it is assumed that also the tangential component of the velocity is continuous. These assumptions lead to the formulation

\[ \frac{Dv}{Dt} = \nabla \cdot T, \quad \nabla \cdot v = 0 \quad \text{in} \quad \Omega \setminus \Sigma(t), \] (3.2)

\[ \llbracket v \rrbracket = 0, \quad V_\Sigma = \langle v, n_\Sigma \rangle \quad \text{on} \quad \Sigma(t), \] (3.3)

\[ V_T = \langle v, n_T \rangle \quad \text{on} \quad \Gamma(t), \] (3.4)

\[ \langle v, n_{\partial \Omega} \rangle = 0 \quad \text{on} \quad \partial \Omega \setminus \Gamma(t), \] (3.5)

where $T = T^T$ is the Cauchy stress tensor. To close the model we consider the energy of the system.

Definition 5. In the simplest case, the total available energy of the system is defined as (see, e.g., [31], [16])

\[ \mathcal{E}(t) := \int_{\Omega \setminus \Sigma(t)} \frac{\rho v^2}{2} dV + \int_{\Sigma(t)} \sigma dA + \int_{W(t)} \sigma_w dA, \] (3.6)

where $W(t) := \Omega^-(t) \cap \partial \Omega$ is the wetted area at time $t$ and $\sigma$, $\sigma_w$ := $\sigma_1 - \sigma_2$ are the specific energies of the fluid-fluid interface and the wetted surface (relative to the “dry” surface).

Assuming constant $\sigma$, $\sigma_w$ with $\sigma > 0$ and $|\sigma_w| < \sigma$ we define an angle $\theta_{eq} \in (0, \pi)$ by the relation

\[ \sigma \cos \theta_{eq} + \sigma_w = 0. \] (3.7)

A direct calculation shows the following result for the energy balance. For a proof see [33], [31].

Theorem 4. Let $\sigma, \sigma_w$ be constant with $\sigma > 0$, $|\sigma_w| < \sigma$ and $\langle v, p, \gamma, \Sigma \rangle$ be a sufficiently regular (classical) solution of the system (3.2) - (3.5). Then

\[ \frac{d\mathcal{E}}{dt} = -2 \int_{\Omega \setminus \Sigma(t)} D : T dV + \int_{\partial \Omega} \langle v, Tn_{\partial \Omega} \rangle dA \]

\[ - \int_{\Sigma(t)} (\|T\| n_\Sigma + \sigma \kappa n_\Sigma) \cdot v dA \]

\[ + \sigma \int_{\Gamma(t)} (\cos \theta - \cos \theta_{eq}) V_T dΓ \] (3.8)

where $D := \frac{1}{2}(\nabla v + \nabla v^T)$ is the rate-of-deformation tensor.

According to the second law of thermodynamics we have to find closure relations such that

\[ \frac{d\mathcal{E}}{dt} \leq 0. \]

3.2 The standard model

Employing the standard closure for the two-phase Navier-Stokes model with constant surface tension, i.e.

\[ T = -p \mathbb{1} + S = -p \mathbb{1} + \eta(\nabla v + (\nabla v)^T), \]

we obtain

\[ \frac{d\mathcal{E}}{dt} = -2 \int_{\Omega \setminus \Sigma(t)} \eta D : D dV + \int_{\partial \Omega} \langle v, S_{n_{\partial \Omega}} \rangle dA \]

\[ + \sigma \int_{\Gamma(t)} (\cos \theta - \cos \theta_{eq}) V_T dΓ. \] (3.9)

Note that the second term vanishes if the usual no-slip condition is kept. However, it is well-known from the literature that this approach does not allow for a moving contact line [22]. Therefore, it is a frequent choice to consider the following generalization.

Remark 6 (Navier slip condition). Assuming that no fluid particles can move across the solid-fluid boundary one still requires $v \cdot n_{\partial \Omega} = 0$ on $\partial \Omega$. In this case, the above term can be rewritten as

\[ \int_{\partial \Omega} \langle P_{\partial \Omega} v, P_{\partial \Omega} S_{n_{\partial \Omega}} \rangle dA. \]

Hence a possible choice to make it non-positive is given by

\[ \langle v, n_{\partial \Omega} \rangle = 0, \quad P_{\partial \Omega} v = -\beta P_{\partial \Omega} S_{n_{\partial \Omega}} \] (3.10)

on $\partial \Omega$ with $\beta \geq 0$. This condition has been first proposed by Navier and relates the amount of tangential slip to the normal stress at the solid boundary. Note that the no-slip condition is recovered in the case $\beta = 0$.  

---

\[ \frac{\sigma}{\sin \theta_{eq}} \text{ Here it is assumed that the fluid particles do not carry angular momentum.} \]
We expect the contact line to advance for incompressible two-phase flows in order to lower the contact angle and to drive the system towards equilibrium.

**Remark 7** (Contact angle boundary condition). It remains to close the last term in (3.9). A sufficient condition to ensure energy dissipation is to require that

$$V_T(\theta - \theta_{eq}) \geq 0. \quad (3.11)$$

This may be achieved by setting

$$\theta = f(V_T) \quad (3.12)$$

with some function $f$ satisfying

$$f(0) = \theta_{eq}, \quad V_T(f(V_T) - \theta_{eq}) \geq 0. \quad (3.13)$$

So, in the absence of external forces, the contact line should only advance if the contact angle is above or equal to the equilibrium value defined by the Young equation (3.2) (and vice versa). This is reasonable if we think of the example of a spreading droplet with an initial contact angle larger than the equilibrium (see Figure 3). We expect the contact line to advance in order to lower the contact angle and to drive the system towards equilibrium.

**Standard model for moving contact lines:** To summarize, we obtained the “standard model for moving contact lines” for incompressible two-phase flows with surface tension in the simplest possible case. This is a purely hydrodynamic model without any transfer processes of heat or mass.

$$\frac{Dv}{Dt} - \eta \Delta v + \nabla p = 0, \quad \nabla \cdot v = 0 \quad \text{in} \ \Omega \setminus \Sigma(t),$$

$$[v] = 0, \quad [p - \mathbb{S}] n_\Sigma = \sigma \kappa n_\Sigma \quad \text{on} \ \Sigma(t),$$

$$\langle v, n_{\partial \Omega} \rangle = 0, \quad \mathbb{P}_{\partial \Omega} v + \beta \mathbb{P}_{\partial \Omega} S n_{\partial \Omega} = 0 \quad \text{on} \ \partial \Omega \setminus \Gamma(t),$$

$$V_T = \langle v, n_T \rangle, \quad \theta = f(V_T) \quad \text{on} \ \Gamma(t).$$

To ensure energy dissipation we further require

$$\eta \geq 0, \quad \beta \geq 0, \quad \sigma \geq 0, \quad V_T(f(V_T) - \theta_{eq}) \geq 0.$$

**The Continuity Lemma:** The following Lemma shows an additional continuity property for the velocity gradient, which only holds at the contact

$$\langle \nabla v, n_{\partial \Omega} \rangle = 0 \Rightarrow \langle \nabla v n_T, n_{\partial \Omega} \rangle = 0.$$

It remains to show that $\langle \nabla v n_T, n_{\partial \Omega} \rangle = 0$. Since $v$ is solenoidal, we have

$$0 = \nabla \cdot v = \langle \nabla v n_T, n_T \rangle + \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle + \langle \nabla v t_T, t_T \rangle.$$

Therefore, we can write

$$\langle \nabla v n_T, n_{\partial \Omega} \rangle = -\langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v t_T, t_T \rangle.$$

From $\tau = -\cos \theta n_T - \sin \theta n_{\partial \Omega}$ we infer (since $0 < \theta < \pi$)

$$n_{\partial \Omega} = -\frac{1}{\sin \theta} (\cos \theta n_T + \tau).$$

This yields

$$\langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle = \frac{1}{\sin \theta} \cos \theta \langle \nabla v n_T, n_{\partial \Omega} \rangle$$

and

$$\langle \nabla v t_T, n_{\partial \Omega} \rangle = \frac{\langle \nabla v t_T, n_{\partial \Omega} \rangle}{\sin \theta} = 0.$$
Note that in the 2D case the full gradient of $v$ is continuous across $\Gamma$. The following corollary provides another way to express the contact angle evolution. All involved quantities are continuous as a consequence of Lemma 1.

**Corollary 1.** Let $\Omega$ be a half-space and $v \in V$ be a velocity field satisfying
\[
\nabla \cdot v = 0 \text{ on } \text{gr } \Omega^\perp, \quad v \cdot n_{\partial \Omega} = 0 \text{ on } \partial \Omega.
\]
Let $gr \Sigma$ be a $C^{1,2}$-family of moving hypersurfaces with
\[
V_{\Sigma} = v \cdot n_{\Sigma} \text{ on } gr \Sigma, \quad V_{\Gamma} = v \cdot n_{\Gamma} \text{ on } gr \Gamma.
\]
Then the evolution of the contact angle is given by
\[
\frac{D\theta}{Dt} = -\sin^2 \theta \langle \nabla v n_{\partial \Omega}, n_{\Gamma} \rangle + \sin \theta \cos \theta \left( \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle \right).
\]
(3.14)

**Proof.** Since $v$ is continuous and $v^\perp \in C^1(\text{gr } \Omega^\perp)$, we can choose $v_{\Sigma} := v^+|_{\text{gr } \Sigma} = v^-|_{\text{gr } \Sigma} \in C^1(\text{gr } \Sigma)$ and apply Theorem 3. Moreover, the vectors $\tau$ and $n_{\Sigma}$ can be expressed as
\[
\tau = -n_{\Gamma} \cos \theta - n_{\partial \Omega} \sin \theta,
\]
\[
n_{\Sigma} = n_{\Gamma} \sin \theta - n_{\partial \Omega} \cos \theta.
\]
(3.15)

The claim follows by inserting (3.15) into equation (2.14) and noticing that
\[
\langle \nabla v n_{\Gamma}, n_{\partial \Omega} \rangle = 0. \quad \square
\]

### 3.3 On the Navier boundary condition

For $\beta > 0$ it is convenient to introduce the friction coefficient $\lambda := 1/\beta$ to write
\[
\langle v, n_{\partial \Omega} \rangle = 0, \quad \lambda P_{\partial \Omega} v + P_{\partial \Omega} S_{n_{\partial \Omega}} = 0. \quad (3.16)
\]
The case $\lambda = 0$ is known as the free-slip condition. Note that in the two-phase case the parameters $\lambda$ and $\eta$ are in general discontinuous across the interface. The quantity
\[
L := \frac{\eta}{\lambda}
\]
has the dimension of a length and is called slip length. If $L$ is strictly positive it may be more convenient to use the inverse slip length
\[
a := \frac{1}{L} = \frac{\lambda}{\eta}.
\]
Note that the slip length may be a function of space and time, i.e. $a = a(t, x)$. Next, we show that the slip length has to be chosen continuously across the contact line to allow for regular solutions.

**Lemma 7.** Under the assumptions of Lemma 5, the tangential part of the Navier condition can be written as
\[
\langle \nabla v n_{\partial \Omega}, n_{\Gamma} \rangle \bigg|_{\Gamma} = -\left( \frac{\lambda}{\eta} \right)^\pm V_{\Gamma},
\]
where the left-hand side is continuous (cf. Lemma 6). Hence to allow for $V_{\Gamma} \neq 0$, the friction coefficients $\lambda^\pm$ have to be chosen such that the slip length is continuous, i.e.
\[
\frac{\lambda^+}{\eta^+} = \frac{\lambda^-}{\eta^-} = a.
\]

In particular, this implies
\[
\lambda^+ = a \eta^+, \quad \lambda^- = a \eta^-, \quad [\lambda] = a [\eta]. \quad (3.17)
\]

**Proof.** We use the fact that the gradient of velocity has additional continuity properties at the contact line (cf. Lemma 3). Because of this, we get from the Navier condition
\[
0 = \lambda^+ \langle v, n_{\Gamma} \rangle + \eta^+ \langle \nabla v + (\nabla v)^T \rangle n_{\partial \Omega}, n_{\Gamma} \rangle
\]
\[
\Leftarrow 0 = \lambda^+ V_{\Gamma} + \eta^+ \langle (\nabla v n_{\partial \Omega}, n_{\Gamma}) + (\nabla v n_{\Gamma}, n_{\partial \Omega}) \rangle = 0
\]

The claim follows by subtracting the two equations at the contact line. \( \square \)

**Corollary 2.** Under the assumption of Corollary 1 let $v$ satisfy the Navier boundary condition (3.16). Then the evolution of the contact angle is given by
\[
\frac{D\theta}{Dt} = \sin(\theta)^2 a V_{\Gamma} + \sin \theta \cos \theta \left( \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle \right).
\]
(3.18)

**Proof.** Employing Lemma 7 to replace $\langle \nabla v n_{\partial \Omega}, n_{\Gamma} \rangle$ in (3.14) proves the claim. \( \square \)

In particular, we observe the following special case for $\theta = \pi/2$.

**Corollary 3.** Under the assumptions of Corollary 3, it holds that
\[
\left. \frac{D\theta}{Dt} \right|_{\theta = \pi/2} = a V_{\Gamma}. \quad (3.19)
\]
Hence $\theta(t) \equiv \pi/2$ implies
\[
0 = a V_{\Gamma}, \quad (3.20)
\]
which means that either $V_{\Gamma} = 0$ or $\lambda = a = 0$.

**Remark 8.** As a consequence, a non-trivial regular solution with $\theta(t) \equiv \pi/2$ is only possible with a free-slip condition ($\lambda = a = 0$). Note that a constant contact angle of $\pi/2$ corresponds to a homogeneous Neumann boundary condition for the level set function. This result confirms the observation from [33], where it is stated that for a regular solution with $a > 0$ and $\theta \equiv \pi/2$ “the point of contact does not move”.
4 Contact angle evolution angle

4.1 Contact angle evolution in the framework of the standard model

The following Theorem shows that $\dot{\theta}$ has a quite simple form for a large class of models. Note that the equations (4.1)–(4.6) say nothing about external forces, do not specify the contact angle and the slip length may be a function of space and time. Moreover, we only need the tangential part of the transmission condition for the stress. In this sense, the system (4.1)–(4.6) is not closed but describes a class of models. The main idea for the proof is the observation that both the Navier and the interfacial transmission condition are active at the contact line. A regular classical solution has to satisfy both of them, which introduces an additional compatibility condition.

**Theorem 5.** Let $\Omega \subset \mathbb{R}^3$ (or $\Omega \subset \mathbb{R}^2$) be a half-space with boundary $\partial \Omega$, $\sigma \equiv \text{const}$, $\eta^\pm > 0$, $[\eta] \neq 0$ and $(v, \text{gr} \Sigma)$ with $v \in \mathcal{V}$, gr $\Sigma$ a $C^{1,2}$-family of moving hypersurfaces with boundary, be a classical solution of the PDE-system

$$\nabla \cdot v = 0 \quad \text{in } \Omega \setminus \Sigma(t),$$

(4.1)

$$[v] = 0, \quad \mathcal{P}_\Sigma [S] n_{\Sigma} = 0 \quad \text{on } \Sigma(t),$$

(4.2)

$$(v, n_{\partial \Omega}) = 0 \quad \text{on } \partial \Omega \setminus \Gamma(t),$$

(4.3)

$$\lambda \mathcal{P}_{\partial \Omega} v + \mathcal{P}_{\partial \Omega} S n_{\partial \Omega} = 0 \quad \text{on } \partial \Omega \setminus \Gamma(t),$$

(4.4)

$$v_{\Sigma} = [v, n_{\Sigma}] \quad \text{on } \Sigma(t),$$

(4.5)

$$v_{\Gamma} = (v, n_{\Gamma}) \quad \text{on } \Gamma(t)$$

(4.6)

and let $0 < \theta_0 < \pi$ be the initial contact angle. Then the evolution of the contact angle is given by

$$\frac{D\theta}{Dt} = \frac{a_{\Gamma}}{2} - \frac{v_{\Gamma}}{2 L},$$

(4.7)

where $a = (\lambda/\eta)^\pm$ is the inverse slip length. Moreover, in the case $\theta = \pi/2$ it holds that

$$(a_{\Gamma})|_{\theta = \pi/2} = 0,$$

which also means that

$$\frac{D\theta}{Dt}|_{\theta = \pi/2} = 0.$$

Proof. The main observation is that both the jump condition and the Navier condition are active at the contact line $\Gamma$. Since $\tau$ is tangential to $\Sigma$, it follows from the continuity of the tangential stress component that

$$\langle [S], n_{\Sigma}, \tau \rangle = 0.$$

Together with the expansions (4.13) for $n_{\Sigma}$ and $\tau$ we obtain

$$0 = -\cos \theta (\sin \theta \langle [S], n_{\Gamma}, \tau \rangle) - \sin \theta (\langle [S], n_{\partial \Omega}, \tau \rangle)$$

$$- \sin \theta (\sin \theta (\langle [S], n_{\partial \Omega}, \tau \rangle) - \cos \theta (\langle [S], n_{\partial \Omega}, \tau \rangle)).$$

Since $S = S^T$ also implies $\langle [S] \rangle = [S]^T$, we get

$$0 = \sin \theta \cos \theta (-\langle [S], n_{\Gamma}, \tau \rangle + \langle [S], n_{\partial \Omega}, \tau \rangle) + (\cos^2 \theta - \sin^2 \theta) \langle [S], n_{\partial \Omega}, \tau \rangle.$$

(4.8)

Since $n_{\Gamma}$ is tangential to $\partial \Omega$, the Navier condition (4.4) implies

$$\lambda^\pm (v, n_{\Gamma}) + \langle S, n_{\partial \Omega}, n_{\Gamma} \rangle = 0.$$

By subtracting the two equations at the contact point, we get (for $0 < \theta < \pi$), using Lemma 7,

$$\langle [S], n_{\partial \Omega}, n_{\Gamma} \rangle = -\lambda V_{\Gamma} = -a V_{\Gamma} \langle [\eta] \rangle.$$

(4.9)

Combining (4.8) and (4.9) we infer

$$0 = \sin \theta \cos \theta (-\langle [S], n_{\Gamma}, \tau \rangle + \langle [S], n_{\partial \Omega}, \tau \rangle) + (\sin^2 \theta - \cos^2 \theta) a v_{\Gamma} \langle [\eta] \rangle$$

(4.10)

on $\Gamma$. Note that for $\theta = \pi/2$ this reduces to

$$a v_{\Gamma} = 0.$$

(4.11)

Hence either $a = 0$ (free-slip) or $v_{\Gamma}$ is zero for $\theta = \pi/2$. To conclude, we simplify equation (4.10). Using Lemma 7 we get

$$\langle [S], n_{\partial \Omega}, n_{\Gamma} \rangle = \langle [\eta] \rangle \langle (\nabla v + (\nabla v)^T) n_{\partial \Omega}, n_{\partial \Omega} \rangle = 2 \langle [\eta] \rangle \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle$$

and with an analogous calculation

$$\langle [S], n_{\Gamma}, n_{\Gamma} \rangle = 2 \langle [\eta] \rangle \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle.$$

Plugging this and (3.17) into equation (4.10) yields

$$0 = 2 \sin \theta \cos \theta \langle [\eta] \rangle \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle + a v_{\Gamma} \langle [\eta] \rangle \langle \sin^2 \theta - \cos^2 \theta \rangle.$$

Using the assumption $[\eta] \neq 0$ we arrive at

$$\sin \theta \cos \theta (\langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle) = -a V_{\Gamma} \langle [\eta] \rangle \langle \sin^2 \theta - \cos^2 \theta \rangle.$$

(4.12)

The claim follows by inserting equation (4.12) into the contact angle evolution equation (3.18):

$$\frac{D\theta}{Dt} = \sin^2 \theta a V_{\Gamma}$$

$$+ \sin \theta \cos \theta (\langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle \nabla v n_{\Gamma}, n_{\Gamma} \rangle)$$

$$= a V_{\Gamma} \left( \sin^2 \theta - \frac{1}{2} \langle \sin^2 \theta - \cos^2 \theta \rangle \right) = \frac{a V_{\Gamma}}{2}.$$  □
Remark 9 (Free Boundary Problem). Following the proof of Theorem 5, it is easy to show that the same result holds for a free boundary formulation, where the Navier-Stokes equations are only solved in the liquid domain. The inviscid gas phase is modeled by a constant pressure field \( p_0 \) and the jump conditions are replaced by

\[
(p_0 - p + S) \eta = \sigma \kappa n \Sigma \quad \text{on} \quad \Sigma(t).
\]

In particular, the viscous stress component \( \langle S \eta \Sigma, \tau \rangle \) vanishes. Due to the Continuity Lemma 6 this also holds for the two-phase problem at the contact line (if \( [\eta] \neq 0 \)), i.e.

\[
0 = \langle [S] \eta \Sigma, \tau \rangle = [\eta] \langle S \eta \Sigma, \tau \rangle \mid _\Gamma.
\]

This turns out to be a very strong condition leading to (4.7).

Corollary 4. Under the assumptions of Theorem 5, a quasi-stationary solution of the model satisfies

\[
aV\tau = 0,
\]

which means that either the contact line is at rest or \( a = 0 \).

Hence non-trivial quasi-stationary solutions only exist for “free-slip”, i.e. \( a = 0 \), but in this case the contact angle is fixed. Conversely, a fixed contact angle with a moving contact line requires free-slip. A more severe problem for the model is the following result.

Corollary 5. Let \( a \geq 0 \) and \( \{v, \eta, \Sigma\} \) be a regular solution in the setting of Theorem 5 that satisfies the thermodynamic condition (3.11). Then (4.7) implies

\[
\dot{\theta} \geq 0 \quad \text{for} \quad \theta \geq \theta_{eq} \quad \text{and} \quad \dot{\theta} \leq 0 \quad \text{for} \quad \theta \leq \theta_{eq}.
\]

With this observation, we can prove that the system cannot evolve towards equilibrium. This clearly shows that the model is unphysical, at least for regular solutions in the sense of Theorem 5.

Corollary 6. Let \( a > 0 \) and \( \{v, \eta, \Sigma\} \) be a regular classical solution of the PDE-system (4.1)-(4.5) in the setting of Theorem 5 that satisfies (3.11). Let the initial condition be such that

\[
\theta(0, x) > \theta_{eq} \quad \forall \quad x \in \Gamma(0),
\]

where \( \Gamma(0) = \partial \Sigma(0) \) is assumed to be bounded. Then it follows that

\[
\theta(t, x) \geq \min_{x' \in \Gamma(0)} \theta(0, x') > \theta_{eq}
\]

for all \( t \in I \cap [0, \infty) \) and \( x \in \Gamma(t) \). That means that the system cannot relax to the equilibrium contact angle.

Proof. Consider \( t \in I \cap [0, \infty) \) and \( x_t \in \Gamma(t) \) arbitrary. Then there exists an \( x_0 \in \Gamma(0) \) such that the unique solution \( x(s) \) of the initial value problem

\[
x'(s) = v(s, x(s)), \quad x(0) = x_0 \in \Gamma(0)
\]

satisfies \( x(t) = x_t \). The point \( x_0 \) can be found by solving (4.14) backwards in time. By integration of (4.7) we conclude

\[
\theta(t, x(t)) = \theta(t, x_t) = \theta(0, x(0)) + \int_0^t \frac{d}{ds} \theta(s, x(s)) \, ds
\]

\[
= \theta(0, x_0) + \int_0^t \frac{aV}{2} \theta(s, x(s)) \, ds
\]

\[
\geq \theta(0, x_0) + \min_{x' \in \Gamma(0)} \theta(0, x') > \theta_{eq}.
\]

Remark 10 (Free-slip condition). Note that a possible solution to the above problem is to postulate free-slip at the contact line (i.e. \( a = 0 \)), which means that

\[
\mathcal{P}_{\theta \Omega} S n_{\theta \Omega} = 0 \quad \text{at} \quad \Gamma(t).
\]

In this case, the contact angle is always equal to \( \theta_{eq} \). This is not necessarily a contradiction to the experimental observations, since the measured “apparent” contact angle may be quite different from the “actual” contact angle in the continuum mechanical model. However, as it is known from experiments and molecular dynamics simulations the slip length in the bulk is typically very small (a few nanometers to a few micrometers for Newtonian liquids [28]).

Remark 11 (Asymptotic solutions and regularity). It is instructive to consider some examples of known asymptotic solutions to wetting flow problems. A classical example is the stationary two-dimensional Stokes problem in the free boundary formulation, i.e. the PDE system

\[
\eta \Delta v = \nabla p, \quad \nabla \cdot v = 0 \quad \text{in} \quad \Omega \setminus \Sigma,
\]

\[
v = 0 \quad \text{on} \quad \Gamma,
\]

\[
\langle v, n_{\partial \Omega} \rangle = 0 \quad \text{on} \quad \partial \Omega \setminus \Gamma,
\]

\[
\lambda \mathcal{P}_{\partial \Omega} v - v_w + \mathcal{P}_{\partial \Omega} S n_{\partial \Omega} = 0 \quad \text{on} \quad \partial \Omega \setminus \Gamma,
\]

\[
\langle v, n_{\Sigma} \rangle = 0 \quad \text{on} \quad \Sigma,
\]

\[
\mathcal{P}_{\Sigma} S n_{\Sigma} = 0 \quad \text{on} \quad \Sigma,
\]

\[
p_0 - p + \langle S n_{\Sigma}, n_{\Sigma} \rangle = \sigma \kappa \quad \text{on} \quad \Sigma,
\]

where \( p_0 \) is the constant outer pressure (see, e.g., [35], [36]). Note that the equations are written in a frame of reference moving with the contact line. So here we have a non-zero tangential wall velocity \( v_w \), which equals the contact line velocity. After introducing the scalar stream function \( \psi \) in polar coordinates \((r, \varphi)\), i.e.

\[
v = v_r \hat{r} + v_\varphi \hat{\varphi}, \quad v_r = \frac{1}{r} \partial_r \psi, \quad v_\varphi = -\partial_\varphi \psi,
\]

(4.22)
the incompressibility condition is automatically satisfied and the pressure can be eliminated from (4.15) leading to the \textit{biharmonic equation}

\[
\Delta^2 \psi = 0 \quad \text{in } \Omega \setminus \Sigma.
\] (4.23)

However, the pressure can be recovered from \( \psi \) via the relations (see \cite{35, 36} for details)

\[
\frac{\partial p}{\partial r} = \left( \frac{1}{r} \frac{\partial^3 \psi}{\partial r^3} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^3} \frac{\partial^2 \psi}{\partial r \partial \varphi} \right) \psi, \quad (4.24)
\]

and

\[
\frac{\partial p}{\partial \varphi} = - \left( \frac{1}{r} \frac{\partial^3 \psi}{\partial r^3} + \frac{1}{r^2} \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r^3} \frac{\partial^2 \psi}{\partial r \partial \varphi} \right) \psi. \quad (4.25)
\]

As a first approximation, the system of equations (4.15)-(4.20) is solved on a wedge domain, i.e. for

\[
0 < r < \infty \quad \text{and} \quad 0 < \varphi < \theta.
\]

 Afterwards, the normal stress condition (4.21) is evaluated to obtain a correction for the free surface shape. Rewriting the boundary conditions (4.16)-(4.20) in terms of the stream function leads to the PDE system

\[
\Delta^2 \psi = 0 \quad \text{for } r > 0, \quad 0 < \varphi < \theta, \quad (4.26)
\]

\[
\psi = 0 \quad \text{for } r \geq 0, \quad \varphi \in \{0, \theta\}, \quad (4.27)
\]

\[
\frac{\partial^2 \psi}{\partial \varphi^2} = 0 \quad \text{for } r > 0, \quad \varphi = \theta, \quad (4.28)
\]

and

\[
\frac{1}{r^2} \frac{\partial^2 \psi}{\partial \varphi^2} + \frac{1}{L} \left( v_w - \frac{1}{r} \frac{\partial \psi}{\partial \varphi} \right) = 0 \quad \text{for } r > 0, \quad \varphi = 0. \quad (4.29)
\]

Moreover, the velocity field is required to be continuous up to the contact point. Since the frame of reference is moving with the contact line, a solution has to satisfy

\[
\lim_{r \to 0} v_r = \lim_{r \to 0} \frac{1}{r} \frac{\partial \psi}{\partial \varphi} = 0. \quad (4.30)
\]

Motivated by a separation of variables approach, one may consider \textit{special} solutions of the type

\[
\psi_\lambda(r, \varphi) = r^\lambda F_\lambda(\varphi). \quad (4.31)
\]

A prominent example of such a solution is the one given by H. K. Moffatt \cite{26}

\[
\psi_1(r, \varphi) = \left( \frac{\varphi - \theta}{\sin \varphi - \varphi \sin(\varphi - \theta) \cos \theta} \right) \left( \frac{\sin \varphi \cos \theta - \varphi \sin \varphi \cos \varphi \cos \theta}{\sin \varphi \cos \theta - \varphi \sin \varphi \cos \varphi \cos \theta} \right),
\]

which satisfies a no-slip condition on \( \partial \Omega \setminus \Gamma(t) \) (for \( v_w = 1 \)). However, the resulting velocity field is discontinuous at the point of contact and the pressure diverges proportional to \( 1/r \), which makes it impossible to satisfy the normal stress condition (4.21) (see \cite{35, 36} for details). In fact, it can be easily seen from (4.22) that for regular \( F_\lambda \neq 0 \), the velocity is continuous on \( \Omega \) if \( \lambda > 1 \). Then condition (4.30) is also satisfied by \( \psi_\lambda \).

Note that for \( \lambda < 2 \) the stress is unbounded for \( r \to 0 \) and Theorem 3 does not apply. For \( \lambda > 2 \) we observe that the tangential stress component vanishes, i.e.

\[
\frac{1}{r^2} \frac{\partial^2 \psi_\lambda}{\partial \varphi^2}(0, 0) = 0.
\]

Using equation (4.29) this implies that either the contact line is at rest or \( L \to \infty \), in agreement with Theorem 3. It follows from the equations (4.24) and (4.25) that \( \lambda > 2 \) is also a sufficient condition to obtain a \textit{finite} pressure at the moving contact line, which is a desirable property from a physical point of view.

![Figure 4: Stream lines for the field given by (4.32).](Image)

It is interesting to take a look at the borderline case \( \lambda = 2 \). For example, the stream function (see \cite{35} and Figure 4)

\[
\psi_2(r, \varphi) = \frac{r^2 v_w}{L_0} \left( -\frac{1}{4} + \frac{\varphi}{\pi} + \frac{1}{4} \cos(2\varphi) \right), \quad (4.32)
\]

describes a velocity field which is an exact solution of (4.26) - (4.30) with \( \theta = \pi/4 \) and a finite slip length \( L_0 \) at the contact point. However, the velocity field is not differentiable at the contact line and the pressure is logarithmically singular. This leads to a correction to the free surface with a singular curvature at the contact point. Due to the lack of differentiability, Theorem 3 also does not apply in this case.

But there are cases for \( \lambda = 2 \), where the required regularity is met. It can be shown that these are given by

\[
\psi_2(r, \varphi) = r^2 (c_1 + c_2 \sin \varphi \cos \varphi + c_3 \sin^2 \varphi),
\]

where \( c_1, c_2, c_3 \in \mathbb{R} \). This class of stream functions represents the (three dimensional) space of \textit{linear} divergence free velocity fields in 2D satisfying \( v = 0 \) at
\[ r = 0. \] The impermeability condition \( v_r = 0 \) for \( \varphi = 0 \) implies \( c_1 = 0. \) The Navier condition \[ 4.29 \] yields
\[ c_3 = -\frac{v_w}{2L_0}, \]
where \( L_0 \) denotes the slip length at the contact point. Finally, the tangential stress condition \[ 4.28 \] allows to determine the constant \( c_2. \) For \( \theta \neq \pi/2 \) we obtain the stream function
\[ \psi_2(r, \varphi) = \frac{v_w r^2}{2L_0} \left( \frac{\sin^2 \theta - \cos^2 \theta}{2 \cos \theta \sin \theta} \sin \varphi \cos \varphi - \sin^2 \varphi \right). \]
The corresponding time derivative of the contact angle is (as expected)
\[ \frac{D\theta}{Dt} = \frac{v_w}{2L_0} \left( \frac{\sin^2 \theta - \cos^2 \theta}{2 \cos \theta \sin \theta} \sin \varphi \cos \varphi - \sin^2 \varphi \right). \]
Clearly, this is not a quasi-stationary solution, i.e. \[ 4.19 \] is not satisfied. As pointed out in Corollary \[ 4. \] a sufficiently regular, non-trivial quasi-stationary solution only exists in the free-slip case.

### 4.2 Empirical contact angle models

The literature contains a large variety of empirical contact angle models, which prescribe the dynamic contact angle. For the simplest class of these models, it is assumed that \( \theta \) can be described by a relation of the type
\[ \theta = f(Ca, \theta_{eq}), \]
where \( \theta_{eq} \) is the equilibrium contact angle given by the Young equation \[ 1.2. \] The capillary number is defined as
\[ Ca := \frac{\eta}{\sigma} \frac{V_T}{\Gamma}. \]
Hence for a given system, \( f \) is a function of the contact line velocity \( V_T, \) i.e.
\[ \theta = f(V_T). \]
If this relation is invertible, one can also write \( (g := f^{-1}) \)
\[ V_T = g(\theta). \]

The following Corollary is an immediate consequence of this modeling.

---

**Corollary 7.** Consider the model described in Theorem \[ 3 \] together with the dynamic contact angle model \[ 4.34. \] Let \( f \in C^1(\mathbb{R}). \) Then, for sufficiently regular solutions, the contact line velocity obeys the evolution equation
\[ f'(V_T) \frac{D}{Dt} V_T = \frac{a V_T}{2}. \]

If the model from Theorem \[ 3 \] is equipped with the contact angle model \[ 4.35 \] with \( g \in C^1(0, \pi), \) the contact angle follows the evolution equation
\[ \frac{D\theta}{Dt} = \frac{a g(\theta)}{2}. \]

**Remark 12.** From Corollary \[ 7 \] we make the following observations.

(i) By taking one of the empirical models \[ 4.34 \] or \[ 4.35 \], we already close the model from Theorem \[ 5 \] for the contact angle evolution and for the evolution of the contact line velocity \( V_T \) (provided that the inverse slip length \( a \) is independent of the state of the system). But note that neither the momentum equation nor the normal part of the transmission condition involving the surface tension is used for the proof. This means that, for regular solutions, neither external forces like gravity nor surface tension forces can influence the motion of the contact line.

(ii) If the empirical functions satisfy the thermodynamic conditions \[ 3.13 \], i.e.
\[ V_T(f(V_T) - \theta_{eq}) \geq 0 \quad \text{and} \quad g(\theta)(\theta - \theta_{eq}) \geq 0 \]
respectively, there are only constant or monotonically increasing/decreasing solutions for \( \theta(t) \) (in Lagrangian coordinates). In addition, the function \( |g'| \) is typically unbounded and the solution exists only on a finite time interval. This is clearly not an acceptable description of the physics of a moving contact line.

(iii) Moreover, we have the additional requirement that \( D_t \theta = 0 \) for \( \theta = \pi/2, \) which dictates \( g(\pi/2) = 0 = g(\theta_{eq}) \) (or \( a = 0 \) which means fixed \( \theta). \)

All these observations together show that one has to consider more complex models in order to obtain regular solutions.

---

### 5 Remarks on possible generalizations

#### 5.1 Marangoni effect

An obvious generalization of the model described in Theorem \[ 3 \] is to include the effect of a non-constant
fluid-fluid surface tension. In this case, the interfacial transmission condition for the stress reads as
\[ [\rho F - S] n_\Sigma = \sigma n_\Sigma + \nabla \Sigma \sigma. \]

**Theorem 6.** Let \( \Omega \subset \mathbb{R}^3 \) (or \( \Omega \subset \mathbb{R}^2 \)) be a half-space with boundary \( \partial \Omega \), \( \eta^2 > 0 \), \( [\eta] \neq 0 \) and \( (v, \gr \Sigma) \) with \( v \in V, \gr \Sigma \) a \( C^{1,2} \)-family of moving hypersurfaces with boundary, be classical solution of the PDE-system
\[
\nabla \cdot v = 0 \quad \text{in} \ \Omega \setminus \Sigma(t),
\]
\[
[v] = 0, \quad P_\Sigma [-S] n_\Sigma = \nabla \Sigma \sigma \quad \text{on} \ \Sigma(t),
\]
\[
\langle v, n_{\partial \Omega} \rangle = 0, \quad \lambda P_{\partial \Omega} v + P_{\partial \Omega} S n_{\partial \Omega} = 0 \quad \text{on} \ \partial \Omega \setminus \Gamma(t),
\]
\[
V_\Sigma = \langle v, n_\Sigma \rangle \quad \text{on} \ \Sigma(t),
\]
\[
V_\Gamma = \langle v, n_\Gamma \rangle \quad \text{on} \ \Gamma(t)
\]
and let \( 0 < \theta_0 < \pi \) be the initial contact angle. Then the evolution of the contact angle is given by
\[
\frac{D \theta}{Dt} = \frac{1}{2} \left( a V_\Gamma - \frac{\partial \sigma}{\partial [\eta]} \right),
\] (5.1)
where \( a = (\lambda/\eta)^\pm \) is the inverse slip length.

**Proof.** Following the proof of Theorem 5, we proceed as follows: From the jump condition for the viscous stress we get
\[
\langle [S] n_\Sigma, \tau \rangle = -\langle \nabla \Sigma, \sigma, \tau \rangle.
\]
Plugging in the expansions for \( n_\Sigma \) and \( \tau \) yields
\[
-\langle \nabla \Sigma, \sigma, \tau \rangle = (\cos^2 \theta - \sin^2 \theta) \langle [S] n_{\partial \Omega}, n_\Gamma \rangle
+ \sin \theta \cos \theta \left( -\langle [S] n_\Gamma, n_\Gamma \rangle + \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle \right).
\] (5.2)
Since the Navier condition is unchanged, we have again (4.9). Combining (5.2) and (4.9) leads to
\[
-\langle \nabla \Sigma, \sigma, \tau \rangle = (\sin^2 \theta - \cos^2 \theta) a V_\Gamma [\eta]
+ \sin \theta \cos \theta \left( -\langle [S] n_\Gamma, n_\Gamma \rangle + \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle \right).
\]
Using Lemma 6, this can be simplified as
\[
\sin \theta \cos \theta \left( -\langle \nabla v n_\Gamma, n_\Gamma \rangle + \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle \right)
= \frac{1}{2} \left( \cos^2 \theta - \sin^2 \theta \right) a V_\Gamma \left[ \frac{\partial \sigma}{\partial [\eta]} \right].
\] (5.3)
The claim follows by inserting (5.3) into the contact angle evolution equation (3.18). \( \square \)

This result resolves the paradox that is found in Theorem 5 since in this case regular solutions with advancing contact line and \( \dot{\theta} < 0 \) are possible. To obtain a non-trivial quasi-stationary state, a surface tension gradient
\[
\partial_\tau \sigma = [\eta] a V_\Gamma
\] (5.4)
has to be present at the contact line. However, for an isothermal system without contamination, there is no obvious reason for non-constant surface tension unless the interface carries additional properties like interfacial mass densities. Then mass fluxes from the bulk to the interface itself have to be included. In this case, the velocity field is no longer continuous at the interface and the interface moves with its own velocity \( v_\Sigma \). Moreover, a physically sound model needs to include full interfacial thermodynamics in a consistent way. This leads for instance to the Interface Formation Model [44].

**Remark 13.** Figure 5(a) shows an example of a linear velocity field satisfying Navier slip with \( L > 0 \) in a co-moving reference frame. The streamlines are tangent to the interface and the contact angle does not change. However, there is a gradient in surface tension according to (5.4). In contrast to that, equation (5.3) implies for \( \theta = \pi/4 \) and constant \( \sigma \) (in the 2D case) that
\[
\langle \nabla v n_\Gamma, n_\Gamma \rangle = \langle \nabla v n_{\partial \Omega}, n_{\partial \Omega} \rangle = 0.
\]
Therefore, the linear part of the velocity field has a quite simple form. In the reference frame of the solid wall, it is given as
\[
(u, v)(x, y) = V_\Gamma \left( 1 + \frac{y}{L} \right).
\]
Figure 5(b) shows the field in a co-moving reference frame. Clearly, the field geometry leads to an increase in the contact angle (clockwise rotation in this example).

### 5.2 Interfacial slip

Another possible generalization of the model is to allow for slip at the fluid-fluid interface. In this case, one only requires continuity of the normal component of the fluid velocity, i.e.
\[
\langle [v] n_\Sigma \rangle = 0 \quad \text{on} \ \Sigma(t),
\]
which means that there is no mass flux from one phase to the other. To describe the evolution of the interface, one can now use both of the fluid velocities
\[
V_\Sigma = \langle v^+, n_\Sigma \rangle, \quad V_\Gamma = \langle v^+, n_\Gamma \rangle.
\]
This gives rise to two distinct Lagrangian derivative operators. Note that the following statement does not require incompressibility of the flow. Therefore, it may also be generalized to analyze models which include phase change between the fluid phases. For simplicity, the theorem is formulated in the case of two spatial dimensions. This ensures that the Lagrangian derivative operators associated with the two fluid velocities coincide at the contact point. A generalization
to three space dimensions is possible by a suitable transformation of the velocities.

**Theorem 7.** Let \( \Omega \subset \mathbb{R}^2 \) be a half-space with boundary \( \partial \Omega, \eta^\pm > 0, [\eta] \neq 0 \) and \( (v, \mathrm{gr} \Sigma) \) with

\[
v \in C^1(\mathrm{gr} \Omega^+) \cap C^1(\mathrm{gr} \Omega^-)
\]

and \( \mathrm{gr} \Sigma \) a \( C^{1,2} \)-family of moving hypersurfaces with boundary, be a classical solution of the PDE-system

\[
\begin{align*}
\mathcal{P}_\Sigma [v - S] n_\Sigma &= \nabla_\Sigma \sigma & \text{on } \Sigma(t), \\
\langle v, n_{\partial \Omega} \rangle &= 0, \quad \lambda \mathcal{P}_{\partial \Omega} v + \mathcal{P}_{\partial \Omega} S n_{\partial \Omega} &= 0 & \text{on } \partial \Omega \setminus \Gamma(t), \\
V_\Sigma &= \langle v^+, n_\Sigma \rangle & \text{on } \Sigma(t), \\
V_\Gamma &= \langle v^+, n_\Gamma \rangle & \text{on } \Gamma(t)
\end{align*}
\]

and let \( 0 < \theta_0 < \pi \) be the initial contact angle. Then the evolution of the contact angle is given by

\[
\frac{D \theta}{Dt} = \frac{1}{2} \left( V_\Gamma \left[ \frac{\partial \sigma}{\partial n} \right] - \frac{\partial \sigma}{\partial n} \right) \tag{5.5}
\]

**Proof.** Since \( v \) is not continuous, Lemma 6 and 7 cannot be used for the proof. We start with the observation, that the two Lagrangian derivatives coincide at the contact line. Since on \( \Gamma \) we have by assumption \( (v^+ - v^-) \cdot n_\Sigma = 0 = (v^+ - v^-) \cdot n_{\partial \Omega} \) and \( n_\Sigma \) and \( n_{\partial \Omega} \) are linearly independent (for \( \theta \in (0, \pi) \)), we still have

\[
[\!v\!]_\Gamma = 0.
\]

Therefore, we observe that

\[
\frac{D^+ \theta}{Dt} |_{\Gamma} = \frac{D^- \theta}{Dt} |_{\Gamma}.
\]

So, at the contact line, we can simply write \( D_t \theta \). Like in Corollary 1, we get

\[
\frac{D \theta}{Dt} = -\sin^2 \theta \langle \nabla v^+, n_{\partial \Omega}, n_\Gamma \rangle \\
+ \sin \theta \cos \theta (\langle \nabla v^+, n_{\partial \Omega}, n_\Omega \rangle - \langle \nabla v^+, n_\Gamma, n_\Gamma \rangle),
\]

where the terms on the right-hand side may now be discontinuous. Using the Navier condition, we can replace the first term

\[
\begin{align*}
\frac{D \theta}{Dt} &= \sin^2 \theta a^+ V_\Gamma \\
+ \sin \theta \cos \theta (\langle \nabla v^+, n_{\partial \Omega}, n_\Omega \rangle - \langle \nabla v^+, n_\Gamma, n_\Gamma \rangle).
\end{align*}
\]

Note that \( a \) may now be discontinuous as well. The next step is to express \( \dot{\theta} \) by means of the jump in normal stress. Thanks to \( \eta^\pm > 0 \) we can write

\[
\begin{align*}
\langle \nabla v^+, n_\Gamma, n_\Gamma \rangle &= \frac{1}{2\eta^+} \langle S^+, n_\Gamma, n_\Gamma \rangle, \\
\langle \nabla v^+, n_{\partial \Omega}, n_{\partial \Omega} \rangle &= \frac{1}{2\eta^+} \langle S^+, n_{\partial \Omega}, n_{\partial \Omega} \rangle.
\end{align*}
\]

Plugging this into the above equation for \( \dot{\theta} \) gives

\[
\begin{align*}
\frac{D \theta}{Dt} &= \sin^2 \theta a^+ V_\Gamma \\
+ \sin \theta \cos \theta \frac{\sin \theta \cos \theta}{2\eta^+} (\langle S^+, n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle S^+, n_\Gamma, n_\Gamma \rangle).
\end{align*}
\]

(5.6)

We introduce \( [S] \) by adding a zero term, i.e.

\[
\begin{align*}
\frac{D \theta}{Dt} &= \sin^2 \theta a^+ V_\Gamma + \frac{\sin \theta \cos \theta}{2\eta^+} (\langle S^+ - S^- \rangle n_{\partial \Omega}, n_{\partial \Omega}) \\
- \langle (S^+ - S^-) n_\Gamma, n_\Gamma \rangle + \langle S^- n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle S^- n_\Gamma, n_\Gamma \rangle).
\end{align*}
\]

(5.7)

Using the second version of the equation (5.6) we have

\[
\sin \theta \cos \theta (\langle S^+, n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle S^+, n_\Gamma, n_\Gamma \rangle) \\
= 2\eta^- \dot{\theta} - 2 \sin^2 \theta a^- \eta^- V_\Gamma.
\]
Together with (5.7) we obtain (using $\lambda^\pm = a^\pm \eta^\pm$)

$$\begin{align*}
\frac{D\theta}{Dt} &= \sin^2 \theta \langle \lambda \rangle V_T \\
&\quad + \frac{\sin \theta \cos \theta}{2} \left( \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle [S] n_{\Gamma}, n_{\Gamma} \rangle \right).
\end{align*}$$

(5.8)

Since $[\eta] \neq 0$ by assumption, we obtained an expression for $\dot{\theta}$ in terms of $[S]$ at the contact line.

Now we exploit the validity of both the Navier and the jump condition for the stress at the contact line. From $P \Sigma [S] n_{\Sigma} = -\partial_r \sigma$ we obtain

$$\langle [S] n_{\Sigma}, \tau \rangle = \sin \theta \cos \theta \left( \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle + \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle \right) + \left( \cos^2 \theta - \sin^2 \theta \right) \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle = -\partial_r \sigma. \quad (5.9)$$

From the Navier condition, i.e.

$$\lambda^\pm V_T + \langle S^\pm n_{\partial \Omega}, n_{\Gamma} \rangle = 0,$$

we infer by taking the trace

$$\langle [S] n_{\partial \Omega}, n_{\Gamma} \rangle = -\langle \lambda \rangle V_T.$$

Combined with (5.9) we obtain

$$\sin \theta \cos \theta \left( \langle [S] n_{\partial \Omega}, n_{\partial \Omega} \rangle - \langle [S] n_{\Gamma}, n_{\Gamma} \rangle \right) = \left( \cos^2 \theta - \sin^2 \theta \right) \langle \lambda \rangle V_T - \partial_r \sigma.$$

Plugging in this expression into (5.8), we finally get

$$\begin{align*}
\frac{D\theta}{Dt} &= \langle \lambda \rangle V_T \left( \sin^2 \theta + \frac{\cos^2 \theta - \sin^2 \theta}{2} \right) - \partial_r \sigma \\
&= \frac{1}{2} \langle \lambda \rangle V_T - \partial_r \sigma.
\end{align*}$$

\[ \square \]

Remark 14. 
(i) If the flow is incompressible and the velocity is continuous, Lemma 7 implies $\langle \lambda \rangle = a [\eta]$ and (5.5) reduces to (5.1).

(ii) In general, it is reasonable to assume that

$$\frac{\langle \lambda \rangle}{[\eta]} \geq 0,$$

which means that both terms have the same sign. Since $\lambda$ can be seen as a friction coefficient, it is reasonable that the more viscous fluid also has the larger $\lambda$. If this is the case, the solutions in the framework of Theorem 7 still show the same unphysical behavior.

5.3 Systems with phase change or interfacial mass

So far we only discussed the case, when no phase transitions occur. In general, there are different kinds of phase transitions as possible generalizations of the model. Given an interface with interface normal field $n_{\Sigma}$ and normal velocity $V_{\Sigma}$, the one-sided mass transfer fluxes are defined as

$$\begin{align*}
\dot{m}^\pm &= \rho^\pm (v^\pm \cdot n_{\Sigma} - V_{\Sigma}), \quad x \in \Sigma(t).
\end{align*}$$

(i) If the interface is not able to store mass, the mass transfer flux has to be continuous, i.e. $[[\dot{m}]] = 0$. In this case, it holds that

$$V_{\Sigma} = v^\pm \cdot n_{\Sigma} - \frac{\dot{m}}{\rho^\pm}.$$

Since the interface is now transported by $V_{\Sigma} \neq v^\pm \cdot n_{\Sigma}$, the mass flux influences the evolution of the interface. In principle, the contact line is now able to move by means of a mass flux from one liquid phase into the other. Physical examples are evaporation and condensation, which give rise to a receding and advancing contact line respectively. Moreover, the mass flux in the contact line region is able to influence the evolution of the contact angle.

(ii) The next logical step to further generalize the model is to allow for $[[\dot{m}]] \neq 0$. Since the total mass still has to be conserved, one then has to consider mass, which is stored on the interface itself. The adsorption and desorption of mass at the interface can be described by an interfacial sorption rate

$$r_{\text{sorp}} + [[\dot{m}]] = 0.$$

Note that the corresponding mass density has to be understood as an \textit{area specific} mass density. Physically, the interfacial mass density can be interpreted as the mass which is stored in a very thin layer making up the interface, where the local density is high due to short range intermolecular forces. In the continuum model, this layer is approximated by a mathematical surface with zero thickness. The presence of interfacial mass gives rise to an additional balance equation, describing the transport of mass within the interfacial layer. The Interface Formation Model introduced by Y. Shikhmurzaev (see \[34\], \[36\]) describes this processes within the framework of continuum thermodynamics of fluid interfaces \[5\], \[4\]. The distribution of mass density determines the surface tension by means of a surface equation of state, which allows predicting the dynamic contact angle as a model output.

Note that, if the solid-liquid interface is able to store mass, the impermeability condition for $v$ does no longer hold, i.e. one may have

$$\langle v^\pm, n_{\partial \Omega} \rangle \bigg|_{\partial \Omega} \neq 0.$$
which allows for a completely different kinematics of the flow. In particular, a “particle” at the fluid-fluid interface is now able to reach the solid wall in finite time. This “rolling motion” is another main feature of the Interface Formation Model, which makes it qualitatively different from the models that we discussed before. Note that there are also models which constitute a simplified version of the Interface Formation Model giving rise to modified boundary conditions, see [25].

The contact angle evolution for this class of models shall be analyzed using the fundamental relation (2.14) in future research.

6 Conclusion

Using the kinematic evolution equation (2.14), we derived the contact angle evolution equation (4.7) which describes the time evolution of the contact angle for sufficiently regular solutions for a class of models based on the two-phase incompressible Navier-Stokes equations in the absence of phase transitions. Together with the usual modeling for the dynamic contact angle respecting the condition (3.11), the contact angle evolution turns out to be unphysical (if the slip length is positive and finite). A gradient in the fluid-fluid surface tension coefficient seems to resolve the problem (5.1). However, it is not obvious where the gradient should come from in the case of an isothermal and clean system. The presence of slip at the fluid-fluid interface also does not change the situation qualitatively (5.5). In view of these results, it seems to be natural to consider models that include interfacial mass densities and/or phase transitions. In particular, the Interface Formation Model seems to be a promising approach in the considered modeling framework.

As a final remark let us note that there are many numerical methods based on the discussed models which, however, do not show the behavior predicted by equation (4.7). In particular, the spreading droplet (cf. Figure 3) is a routinely used test case for numerical methods. The equilibrium shape is known (see [13]) and can be compared to the numerically obtained stationary state. According to equation (4.7), it is impossible to reach the equilibrium contact angle with a regular velocity field. There are different possible reasons why this behavior is not observed.

(i) If we assume that there is a unique solution to the PDE system in some larger function space, then the numerical method may indeed correctly approximate a velocity field that shows a (weak) singularity at the contact line. Theorem 3 does not apply in this case. But note, that for such a velocity field the pure advection problem

$$\partial_t \phi + v \cdot \nabla \phi = 0$$

is typically not uniquely solvable because the ODE for the trajectories

$$\dot{x}(t) = v(t, x(t))$$

is not uniquely solvable. Therefore, it is not trivial to obtain convergence of the numerical solution. As it is shown in [10], already the Bi-Laplace equation in a wedge, i.e. the equation

$$\Delta^2 \psi = 0,$$

which is considered as fundamental for the moving contact line problem, is not uniquely solvable with the usual boundary conditions. Instead, there are “undesired solutions”, which have to be ruled out by the numerical method, see [10] for details. Essentially, the numerical method has to include some a priori knowledge about the singularity in order to handle it in a feasible way.

(ii) Many methods use some kind of algorithm to “correct” or “adjust” the contact angle after a transport step according to the desired contact angle model. Once this is done, the evolution of the contact angle is no longer consistent with the flow and the obtained discrete solutions cannot be expected to approximate a regular solution to the underlying continuous PDE model.

(iii) Many numerical methods use a one-field formulation of the two-phase Navier-Stokes system based on the Continuum Surface Force (CSF) approach by Brackbill, Kothe and Zemach [10]. In this formulation, the interfacial transmission conditions for the stress are dropped in favor of a volumetric force term in the momentum balance, which is supposed to model the effect of surface tension. The advantage of this approach is that the momentum equation can be solved on the whole domain using averaged coefficients for the physical properties like density and viscosity and an additional force term. However, it is not clear why the continuity of the tangential stress component, i.e.

$$\langle [S] n_{\Sigma}, \tau \rangle = 0,$$

should still hold. But the validity of this condition at the contact line is a crucial ingredient for the proof of (4.7).
All these observations indicate that it may be desirable to look for modified models allowing for physically reasonable regular solutions. The complementary approach is to further study the singularity and develop numerical methods which are able to handle it.

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A Appendix

Lemma A.1 (Separated local parametrization). Let \( \{ \Sigma(t) \}_{t \in I} \) be a \( C^{1,2} \)-family of moving hypersurfaces and \((t_0, x_0)\) be an inner point of \( M = \text{gr} \Sigma \). Then there exists an open neighborhood \( U \subseteq \mathbb{R}^4 \) of \((t_0, x_0)\), \( \delta, \epsilon > 0 \) and a \( C^1 \)-parametrization

\[
\phi : (t_0 - \delta, t_0 + \delta) \times B^2_\delta(0) \to M \cap U
\]

of \( M \) such that \( \phi(t_0, 0) = (t_0, x_0) \) and

\[
\phi(t, \cdot) : B^2_\delta(0) \to \{t\} \times \Sigma(t)
\]

is a \( C^2 \)-parametrization of \( \Sigma(t) \). In particular

\[
\phi(t, u) = (t, \hat{\phi}(t, u)),
\]

with a \( C^1 \)-function \( \hat{\phi} \).

Proof. By definition of a \( C^{1,2} \)-family of moving hypersurfaces, there is \( \eta > 0 \) and an open neighborhood of \((t_0, x_0)\) in \( \mathbb{R}^4 \) and a local \( C^1 \)-parametrization

\[
\psi = (\psi_1, \psi_2) : \mathbb{R}^3 \cap B^3_\eta(0) \to \text{gr} \Sigma \cap U \quad (A.1)
\]

such that \( \psi(0) = (t_0, x_0) \) and \( \psi(x) \in \Sigma(\psi(t)) \) for all \( u \in B^3_\eta(0) \). The goal is to find a coordinate transformation

\[
T : I_\delta(t_0) \times B^2_\delta(0) \to B^3_\eta(0)
\]

such that

\[
\phi(T(s, y_1, y_2)) = s.
\]

Since \( \psi \) is injective, there is \( i \in \{1, 2, 3\} \) such that

\[
(\partial_{u_i} \psi_2)(0, 0, 0) \neq 0, \quad (A.2)
\]

where we may assume \( i = 1 \). We now choose a special function \( T \) of the form

\[
T(s, y_1, y_2) = (\varphi(s, y_1, y_2), y_1, y_2)
\]

and look for a function \( \varphi \) satisfying

\[
\psi_1(\varphi(s, y_1, y_2), y_1, y_2) = s
\]

\[
\Leftrightarrow 0 = f(s, y_1, y_2; \varphi(s, y_1, y_2)).
\]

The \( C^1 \)-function \( f(s, y_1, y_2; \varphi) := \psi_1(\varphi, y_1, y_2) - s \) satisfies \( f(t_0, 0, 0) = 0 \) and \( \nabla f \) implies

\[
\partial_x f(t_0, 0, 0) \neq 0.
\]

Now the claim follows by the Implicit Function Theorem.

Note that exactly the same procedure yields a \( C^1 \)-parametrization of the submanifold \( \text{gr} \Sigma \) of the form

\[
\phi : (t_0 - \delta, t_0 + \delta) \times (-\epsilon, \epsilon) \to \text{gr} \Sigma \cap U
\]

such that \( \phi(t_0, \cdot) \) is a \( C^1 \)-parametrization of \( \Sigma(t_0) \). As a consequence of that, we can give an explicit characterization of the tangent spaces of \( \text{gr} \Sigma \) and \( \text{gr} \Gamma \).

Lemma A.2 (Tangent spaces). The tangent space of \( \text{gr} \Sigma \) at the point \((t, x)\) is given by

\[
T_{\text{gr} \Sigma}(t, x) = \{ \lambda (1, V \Sigma n_{\Sigma}(t, x)) + (0, \tau) : \lambda \in \mathbb{R}, \tau \in T_{\Sigma(t)}(x) \}.
\]

Likewise, the tangent space of \( \text{gr} \Gamma \) at the point \((t, x)\) is given by

\[
T_{\text{gr} \Gamma}(t, x) = \{ \lambda (1, V \Gamma n_{\Gamma}(t, x)) + (0, \tau) : \lambda \in \mathbb{R}, \tau \in T_{\Gamma(t)}(t, x) \}.
\]

Proof. We make use of the parametrization constructed in Lemma A.1.

For \((t_0, x_0)\) in \( \text{gr} \Sigma \) choose a \( C^1 \)-parametrization

\[
\phi : (t_0 - \delta, t_0 + \delta) \times B^2_\delta(0) \to M \cap U,
\]

\[
\phi(t, u_1, u_2) = (t, \hat{\phi}(t, u_1, u_2))
\]

such that \( \phi(t_0, 0, 0) = (t_0, x_0) \). A basis for the tangent space \( T_{\text{gr} \Sigma}(t_0, x_0) \) is then given by

\[
\{ \partial_t \phi(t_0, 0, 0), \partial_{u_1} \phi(t_0, 0, 0), \partial_{u_2} \phi(t_0, 0, 0) \} = \{ (1, \partial_t \hat{\phi}(t_0, 0, 0), 0, \partial_{u_1} \hat{\phi}(t_0, 0, 0)),
\]

\[
(0, \partial_{u_2} \hat{\phi}(t_0, 0, 0)) \}
\]

where the vectors

\[
v_1 := \partial_{u_1} \hat{\phi}(t_0, 0, 0) \quad \text{and} \quad v_2 := \partial_{u_2} \hat{\phi}(t_0, 0, 0)
\]

constitute a basis of \( T_{\Sigma(t_0)}(x_0) \). By definition of the normal velocity \( V_{\Sigma} \), we have

\[
\partial_t \hat{\phi}(t_0, 0, 0) = \left( \partial_t \hat{\phi}(t_0, 0, 0), n_{\Sigma}(t_0, x_0) \right) n_{\Sigma}(t_0, x_0)
\]

\[
+ \mathcal{P}_{\Sigma} \partial_t \hat{\phi}(t_0, 0, 0)
\]

\[
= V_{\Sigma}(t_0, x_0)n_{\Sigma}(t_0, x_0) + \mathcal{P}_{\Sigma} \partial_t \hat{\phi}(t_0, 0, 0).
\]
Since the second term can be expressed in terms of \( v_1 \) and \( v_2 \), we obtain a basis of the desired form
\[
\{(1, V_T(t_0, x_0)w(t_0, x_0)), (0, \partial_{u_1} \phi(t_0, 0, 0)), (0, \partial_{u_2} \phi(t_0, 0, 0))\}.
\]

For \((t_0, x_0) \in \Gamma_T\) choose a \( C^1 \)-parametrization
\[
\phi : (t_0 - \varepsilon, t_0 + \varepsilon) \times (-\varepsilon, \varepsilon) \rightarrow \Gamma_T \cap U,
\phi(t, u) = (t, \phi(t, u)),
\]
such that \( \phi(t_0, 0) = (t_0, x_0) \). The same procedure as above shows that the set
\[
\{(1, V_T\Gamma_T(t_0, x_0)), (0, \partial_u \phi(t_0, 0))\}
\]
is a basis of the Tangent space \( T_{\Gamma_T}(t_0, x_0) \), where
\( \partial_u \phi(t_0, 0) \) is a basis of \( T_{\Gamma_T}(t_0, x_0) \).

\[\square\]

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