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## **Erklärung zur Abschlussarbeit gemäß §22 Abs. 7 und §23 Abs. 7 APB der TU Darmstadt**

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Hiermit versichere ich, Jan Kröger, die vorliegende Masterarbeit ohne Hilfe Dritter und nur mit den angegebenen Quellen und Hilfsmitteln angefertigt zu haben. Alle Stellen, die Quellen entnommen wurden, sind als solche kenntlich gemacht worden. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen.

Mir ist bekannt, dass im Fall eines Plagiats (§38 Abs. 2 APB) ein Täuschungsversuch vorliegt, der dazu führt, dass die Arbeit mit 5,0 bewertet und damit ein Prüfungsversuch verbraucht wird. Abschlussarbeiten dürfen nur einmal wiederholt werden.

Bei der abgegebenen Thesis stimmen die schriftliche und die zur Archivierung eingereichte elektronische Fassung gemäß §23 Abs. 7 APB überein.

Bei einer Thesis des Fachbereichs Architektur entspricht die eingereichte elektronische Fassung dem vorgestellten Modell und den vorgelegten Plänen.

Darmstadt, 11. Oktober 2023

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J. Kröger

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# 1 Introduction

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Many everyday phenomena that we observe are, contrary to expectations, not yet fully understood. This does not mean that they are not utilized in a variety of technical devices. In the case of wetting, we encounter many different things in everyday life, such as a drop on a window pane that seems to slide down randomly, or the sleeve of a sweater that seems to soak up water when washing hands.

Nature has a head start in this effect and has produced creatures that can walk on water because they take advantage of the water's surface tension. The flora also uses surface tension, whether it's trees that wouldn't reach the size we know without the capillary effect, or the lotus flower, which, with its water-repellent (hydrophobic) surface, ensures that water rolls off and takes dirt with it in the process.

Porous media, through their use in oxygenators, became lifesavers during the Corona pandemic by reoxygenating blood. The potential applications and necessities of this phenomenon could be demonstrated with many more examples. This work aims to describe the dynamics of capillary rise through simulations. A porous medium can be simplified as a collection of many small tubes. Insights from these small tubes can then be extrapolated to determine the behavior of the porous medium. Therefore, experiments with both porous media and individual capillaries are of great interest to understand how the rise in the capillary is designed. Simulations of these processes are also increasingly being carried out, as they have the advantage of fixing certain relevant material properties to examine their influence, or to look into areas that would not be possible with a conventional experimental setup.

In this work, the rise of a liquid column (water) in a capillary is investigated. Specifically, for a two-phase system, the area around the interface in the water phase is examined, and how dissipative processes in this region influence the rise of the water column. Possible phase changes (evaporation, boiling, condensation, etc.) are not taken into account. An isothermal and isobaric system is also assumed. All fluids treated are Newtonian, and the flow can be assumed to be Poiseuille flow. Furthermore, newly implemented boundary conditions of the used solver, which are supposed to better represent the behavior of the contact line and contact angle, will also be checked.

This work will first discuss important findings in the description of capillary rise, the contact line, and the simulation of such problems with phase field methods in Chapter ???. This is followed by an overview of the important influencing factors of wetting and

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their influence on the topics discussed in Chapter 2. Chapter 3 provides an introduction to the phase field method and how it is implemented to simulate such problems. Chapter 5 shows that the solver used has already shown in many other simulations that it produces correct results and is applicable to these problems. Validation of the geometries used here is not possible due to their size, as they have a radius of 3 nm. It is not currently known that there are experiments that provide reliable results with a constant cross-section and such small radii. Subsequently, Chapter 4 describes the setup of the simulations with descriptions of the geometry, material properties used, and solver settings. Finally, the results are discussed in Chapter , and an outlook for upcoming investigations is given in Chapter .

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The solver used here is `phaseFieldFoam`, which is an extension of the open-source environment `OpenFOAM-extend`. The version used of `OpenFOAM-extend` is 5.0, and the version of the solver is still in development. The further development and maintenance of the solver are carried out through a cooperation between KIT (Karlsruhe Institute of Technology) and TU Darmstadt, especially by Dr.-Ing. Xuan Cai and Dr.-Ing. Holger Marschall. The simulations for this research were conducted on the Lichtenberg high-performance computer of the TU Darmstadt.

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The dynamics of a rising fluid in the capillary is the subject of many processes. In nature, for example, trees would not be able to grow as high as they do without the capillary effect, and in technology many processes with a porous medium exist. Porous media can be simplified as many small tubes through which a fluid travels. Therefore, this process has long been of great interest in science and yet there are many uncertainties in the description of the dynamics.

The Lucas Washburn equation, introduced in 1921 [[lucas\\_ueber\\_1918](#), [washburn\\_dynamics\\_1921](#)], attempts to describe the height of the propagating fluid column as a function of time. This equation is sufficiently accurate for many applications.

However, due to the assumptions made in the derivation of the equation, it is clear that it cannot be applied to every problem. Therefore, there are many approaches to adapt this equation to problems and simply maintain the behaviour of the equation.

It is shown, that the Lucas Washburn equation has its problems in early stages of the imbibition [[bosanquet\\_lv\\_1923](#), [quere\\_inertial\\_1997](#)], due to the undefined behaviour for  $t = 0$  and neglecting the inertia of the fluid.

The early stages of the imbibition process is yet to be understood and in this work we show how the different forces are acting on the meniscus for small time steps with a simulation of the such a problem. This simulations are done with the open source framework of `foam extend`, which is a fork of `open foam`. Here the department of mathmatics of the TU Darmstadt and the KIT developed a solver for a phase field approach.

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The developed solver phaseFieldFoam is maintained and developed by the department of MMA at the Tu darmstadt and ... KIT. It is using the Phase field approach to solve the Navier Stokes Equations (NSE).

In this work, first the attempts to describe the imbibition of a fluid in a capillary, especially for the early stages and small capillaries are discussed. Followed by the work, which has been done to simulate such problems with the phase field approach. Important interrelationships and derivations of the process of wetting is discussed, again followed by the equivalent numerical relations. How the simulations are setup and the results are in the chapters and .

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## 2 Wetting Theory

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The wetting theory describes the interaction of fluids with solid surfaces. Many processes in nature, as well as in technology, are affected by this phenomenon. In this work, the focus is on the wetting properties in capillaries, which are often used as a simplification for understanding porous media or in other processes, such as the fact that trees would not be as tall as they are today without this effect.

First, an overview of some types of wetting is presented , and the concepts of contact angle and contact line are introduced. Subsequently, the surface tension and its role in wetting are discussed. Since this work considers the dynamic rise of a water column in a capillary, the dynamic contact angle is also examined in Chapter , followed by a description of the capillary effect and its significance for the rise of a fluid in a capillary.

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### 2.1 Surface Tension

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Surface tension plays a significant role in the wetting of surfaces or in capillary rise. Therefore, it is essential to first clarify what surface tension is. In general, surface tension is a proportionality constant that depends on temperature, pressure, and the phases involved but is independent of the surface [5]. The interface separates the phases and can be interpreted differently. On a molecular level, molecules attract each other (cohesion). The interaction between two phases is called adhesion. In the case of the interaction between a liquid and a solid, adhesion can usually be neglected. In Figure 2.1, a water droplet surrounded by air is illustrated on the left. The black outer line thus represents the interface between the droplet and the air. If one now magnifies the transition area down to the molecular level (red area), one obtains the schematic representation on the right side. The blue circles are simplified representations of the water molecules, and the gray ones represent the surrounding air. Here, it is evident how, at the interface, the water molecules are no longer surrounded only by other water molecules, which is energetically unfavorable. However, since the system strives to transition into an energetically favorable state, it attempts to minimize the number of molecules lying at the interface [5].

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To increase the surface area, molecules must be transported to the surface, and energy must be supplied to the system. Therefore, surface tension is also interpreted as the



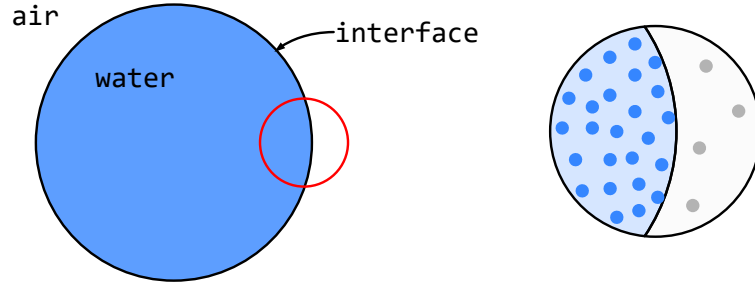


Figure 2.1: Schematic of interacting molecules in a liquid droplet and its interaction with a vapor

necessary energy required to carry a molecule to the surface.

$$dE = \sigma \cdot dA \quad (2.1)$$

with  $dE$  as the supplied energy and  $dA$  as the change in surface area.

## 2.2 Wetting Phenomenon

Despite the fact that the wetting of droplets is not considered in this work, it is appropriate to describe the fundamentals of wetting using this example. The concepts are the same, and many initial studies are based on this example.

In the case where the system is in equilibrium, Young derived an equation relating surface tensions to the contact angle:

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$$\sigma_{LV} \cdot \cos \theta_e = \sigma_{SV} - \sigma_{SL} \quad (2.2)$$

Where  $\sigma_{LV}$  is the surface tension between the liquid and the gas,  $\sigma_{SV}$  is from the solid to the gas, and  $\sigma_{SL}$  is between the solid and the liquid (see Figure 2.2). If  $(\sigma_{SV} > \sigma_{SL})$  holds true, a contact angle less than  $90^\circ$  follows; otherwise,  $90^\circ \leq \theta_e < 180^\circ$ . In the case where  $\sigma_{SV} = \sigma_{SL} + \sigma_{LV}$ , complete wetting of the surface occurs [5].

When a droplet impacts a solid surface, different states can arise depending on the fluid-solid combination. At the point where the interface of the two fluids (droplet and surrounding fluid) meets the solid surface, the contact line is formed (see 2.2; red line). Depending on the fluid-fluid-solid combination, a contact angle  $\theta_e$  is established, where the suffix  $e$  stands for equilibrium. In the case of complete wetting, the fluid spreads over the entire surface (see Figure 2.3 a)). This effect, however, is challenging to reproduce as it can be hindered by surface irregularities [5]. As seen in Figure 2.3(b-d)), states where a droplet forms on the surface are further subdivided. For a contact angle  $\theta_e < 90^\circ$ , it is

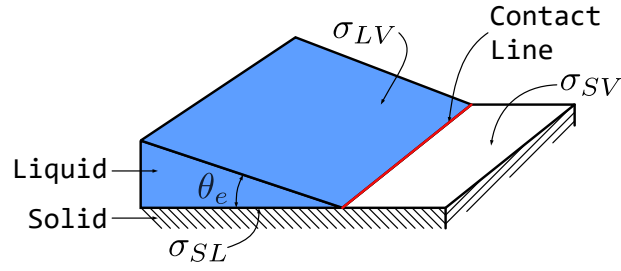


Figure 2.2: Three Phase Contact Line

termed hydrophilic (see 2.3b)), for  $\theta_e > 90^\circ$  it's hydrophobic (see 2.3c)), and for a contact angle  $\theta_e > 120^\circ$ , it's superhydrophobic surfaces (see 2.3d)). Developing superhydrophobic surfaces is also challenging. To curve the surface of the liquid, a pressure difference must

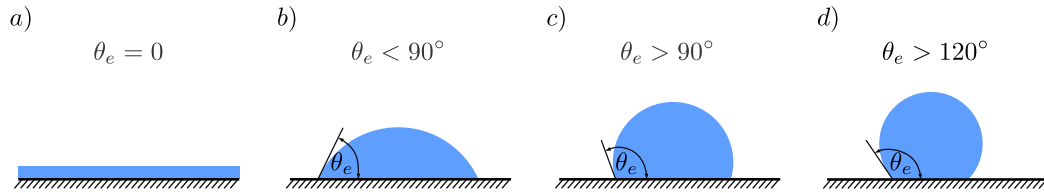


Figure 2.3: Wetting of a surface

exist. In the case of a sphere, Young and Laplace developed a relationship for the pressure difference in terms of the surface tension and radius as:

$$P_i - P_o = \Delta P = \frac{2\sigma}{R} \quad (2.3)$$

With  $\Delta P$  being the pressure difference at the interface,  $P_i$  as the pressure inside the droplet,  $P_o$  the ambient pressure, and  $R$  as the radius of the sphere. For a derivation, refer to [5].

### 2.2.1 Dynamic Weting

So far, only states have been considered that observe systems in equilibrium. Typically, however, the contact line is in motion. When the contact line is moving, the contact angle (dynamic contact angle  $\theta_D$ ) differs from that in the equilibrium state [3]. To describe the dynamics of the contact line, the dynamic contact angle, the relative speed of the contact line, and the equilibrium contact angle are required [32, 3, 12, 24, 39]. However, describing the contact line is challenging due to the fact that the microscopic level affects the macroscopic level.

In Figure 2.4, various views of the contact line are illustrated. The red circle in a) points to the area considered in the picture next to it and can be understood as a magnifying glass. If we enlarge the area in a), we see the interpretation of the contact line from the perspective of the hydrodynamic theory, with a microscopic contact angle  $\theta_m$  and the dynamic contact angle  $\theta_D$  (Figure 2.4 b)). Focusing again on the contact line, we see the interpretation of the molecular kinetic theory (Figure 2.4 c)). The illustrated points are intended to represent molecules in a simplified form.

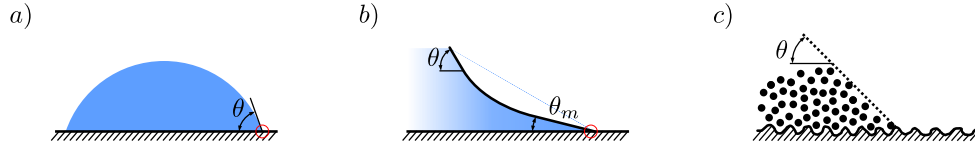


Figure 2.4: Hydrodynamic and Molecular Kinetic description of the Contact angle. Figure b) corresponds to the area circled in red in a), and c) to the area from image b).

**Hydrodynamic Theory** The hydrodynamic approach solves the physics of the flow using the Navier-Stokes equations but encounters a singularity at the contact line when a sticking condition is applied [24]. To address this issue, either the sticking condition near the wall was relaxed or the solution was truncated at the molecular level [3]. In both cases, a small capillary number is assumed, which means that far from the contact line, the interface assumes its equilibrium shape.

Voinov [39] derived a description of the contact line for a spreading droplet depending on the capillary number. A generalized version was developed by Cox [12] with some correction terms [9, 3]. Thus, the dynamic contact angle for  $\theta_D \leq 3/4\pi$  is given by

$$\theta_D^3 - \theta_m^3 = 9Ca \ln \left( \frac{L}{L_m} \right) = 9 \frac{\mu u}{\sigma} \ln \left( \frac{L}{L_m} \right) \quad (2.4)$$

With  $L$  as the macroscopic path length and  $L_m$  as the microscopic path length. Assuming that the interface assumes its equilibrium shape far away,  $\theta_m = \theta_e$ . However, Voinov himself already pointed out that  $\theta_m$  could also depend on the speed [39, 3].

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**Molecular Kinetic Theory** The Molecular Kinetic Model describes the movement of the contact line with a statistical description of the molecular movement at the contact line [2]. In contrast to the hydrodynamic model, the molecular processes at the contact line influence those of the larger scales. In this view, the molecules at the contact line jump back and forth to adsorption sites on the solid substrate. The speed of the contact line is determined by multiplying the difference between the forward and backward jumps by a

jump distance  $\lambda$ . This results in the description

$$u = 2\lambda\kappa_0 \sinh\left(\frac{\sigma(\cos\theta_e - \cos\theta_D)}{2nk_B T}\right). \quad (2.5)$$

Where  $n$  is the number of adsorption sites per unit area,  $\kappa_0$  is a characteristic frequency,  $k_B$  is the Boltzmann constant, and  $T$  is the temperature. If the system is in equilibrium, the forward and backward jumping is balanced, and the contact line comes to a standstill [8, 3]. However, a problem with this view is that this model is more qualitative and computationally intensive [32].

### 2.2.2 Capillary Rise

A capillary is a very thin tube in which, due to surface effects, a liquid rises or falls without external force. In 2.5, a capillary with an already risen liquid column is shown. The well-known surface tensions are also marked at their respective locations, as well as the essential geometric parameters, such as diameter ( $2R$ ) or height of the resulting meniscus  $z$ . The resulting contact angle after reaching equilibrium,  $\theta_e$ , is also shown. The system in this representation is also subject to gravitational forces.

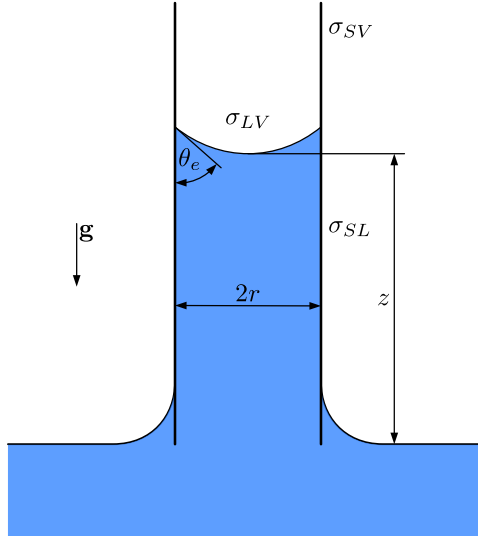


Figure 2.5: Schematic representation of a capillary in a liquid after it has penetrated the capillary.

In this work, such a system is used. However, further conditions apply. It is assumed that the system is isobaric, isothermal, and the liquid is Newtonian. Furthermore, it is assumed that while the water column rises in the capillary, a Poiseuille flow is present and no phase

change occurs. It is also assumed that the viscosity of the gas phase is negligible. With these assumptions and boundary conditions, the Newtonian dynamics in a capillary can be described as a balance between the inertial forces and the sum of the capillary forces, viscous forces, and hydrostatic forces [18]:

$$\frac{d}{dt}M(z, \dot{z}) = F_w - F_\eta - F_g \quad (2.6)$$

With  $M(z, \dot{z}) = \pi r^2 \rho z \dot{z}$  as the moment,  $F_g = \pi r^2 \rho g z$  as the gravitational force, and  $F_\eta$  as the viscous resistance, which results from the assumption of the average velocity and the existing Poiseuille flow to  $F_\eta = 8\pi\eta z \dot{z}$ . With  $\dot{z}$  as the average velocity. The capillary forces result from the previous description of the surface tension and the change in the surface of the meniscus with a change in the current height:

$$F_w = \sigma \frac{dA}{dz} = \sigma 2\pi r \quad (2.7)$$

The surface tension  $\sigma$  here is the increase in surface energy due to the wetting of the solid wall of the capillary. Thus,  $\sigma = \sigma_{SV} - \sigma_{SL}$ . This description is already known from the Young equation (2.2). Thus, after inserting for the capillary forces:

$$F_w = \sigma_{LV} \cdot \cos \theta_e 2\pi r. \quad (2.8)$$

Thus, for equation 2.6 after insertion [18]:

$$\pi r^2 \rho \frac{d}{dt}(z \dot{z}) = \sigma_{LV} \cdot \cos \theta_e 2\pi r - 8\pi\eta z \dot{z} - \pi r^2 \rho g z. \quad (2.9)$$

Early descriptions by Bell and Cameron [1] did not describe the rise dynamics based on equation 2.9. They developed the rise dynamics from experiments according to:

$$z(t)^n = K \cdot t. \quad (2.10)$$

Both  $n$  and  $K$  are temperature-dependent constants. In 1918, Lucas [30] and in 1921, Washburn [40] derived the Lucas Washburn equation by neglecting the inertial and gravitational terms:

$$z(t) = \sqrt{\frac{r \sigma \cos \theta_e}{2\eta}} t \quad (2.11)$$

With this, they independently developed an equation with which the capillary rise can be described based on material values and measurements. Therefore, it gained popularity

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over the years. Due to the neglect of individual terms and simplifications in the system, however, this equation is not always precise for several reasons. Washburn himself pointed out that to meet the prediction of the equation, he had to set up the experiments in such a way that the capillary was prewetted. Therefore, adjustments to this equation were made for various problems [15, 22, 6, 19, 18, 14, 31]. Wu et al. [41] examined several models and compared them with experiments. In these, however, it is always assumed that the height of the meniscus increases according to  $z(t) \sim \sqrt{t}$  as well.

Bosanquet [4] hinted in his 1923 paper that equation 2.11 would lead to unphysical behavior for  $t \rightarrow 0$  and also developed an equation that retained this problem but now also included inertia and can give a better prediction of the rise for early times of imbibition, but also fails for small capillary [11].

Siegel [36] studied the rise behavior under microgravity and found a linear growth. However, he did not reach the Lucas-Washburn regime. Zhmud et al. [45] also pointed out the problems for times near 0 from equation 2.11 and described a quadratic relationship for the times when the fluid is drawn into the capillary, followed by the known Lucas-Washburn regime.

Dreyer et al. [17] studied parallel plates under microgravity and divided the rise of the meniscus into three regions. Starting with a quadratic growth, followed by a linear region, and finally the Lucas-Washburn growth. Quéré [34] showed a linear growth at the beginning by assuming that in this case only inertia plays a role. Stange [37] confirmed the three regions of Dreyer et al. [17] and derived dimensionless equations to develop transition times.

Fries et al. [20] divided the growth area into areas where different forces act. In the beginning, inertia dominates, followed by a transition area where the viscous forces take over until they finally dominate. They also developed dimensionless times at which the transition takes place.

At the point where the viscous friction and the effects of inertia or dynamic contact angle are equal, Quéré [34] and Fries et al. [20] defined the characteristic penetration length:

$$l_c \propto r \sqrt{\frac{r \rho \sigma}{\mu^2}} \quad (2.12)$$

Dellano et al. [14] focused on early times and studied viscous fluids, confirming the influence of pre-wetting the capillary, as already mentioned by Washburn [40]. They also showed a deviation from the Lucas-Washburn regime at early times. They attributed this deviation to local viscous dissipation in the wedge region, rather than a global dissipation as assumed by Lucas and Washburn. Regarding the dynamic contact angle, they showed that the characteristic penetration length (cf. Equation 2.12) is calculated as:

$$l_c \propto r \ln \left( \frac{r}{l_m} \right) \quad (2.13)$$

With  $l_m$  being the microscopic length that compensates for the singularity of the contact line [12]. They further assumed that once  $l_c$  is reached, the transition to the Lucas-Washburn regime occurs.

Ruiz-Gutiérrez et al. [35] contradicted this statement in their work, showing that this transition takes longer. They argue that the effects of inertia and dynamic contact angle do not decay exponentially.

To account for this, they expanded Equation 2.9 for problems with a moving interface by introducing:

$$f(\dot{z}) \equiv \frac{\cos \theta_m - \cos \theta_D(\dot{z})}{\cos \theta_m} \quad (2.14)$$

With the assumption that for  $u > 0$  from Equation 2.4,  $\theta_D > \theta_m$  holds true, this function disappears for  $\theta_D \rightarrow \theta_m$ .

Now, considering the moving system, Equation 2.9 for the case studied in this work becomes:

$$\pi r^2 \rho z \frac{du}{dt} = 2\pi r \sigma \cos \theta_m + \pi r^2 \rho g z - 8\pi \sigma z \dot{z} - 2\pi r \sigma \cos \theta_m f \quad (2.15)$$

With the first two terms as driving forces and the last two as resistance forces. The last term has been added and acts as a correction for the fact that the dynamic contact angle does not correspond to the macroscopic contact angle.

Subsequently, dimensionless quantities were introduced, and four cases were defined. Two each with a large and small Laplace number, or a large and small ratio of length scales. With the quantities used in this work, case three from Ruiz-Gutiérrez et al. [35] should apply. They predict that the quadratic regime will not occur, and the rise will begin with a linear region, eventually transitioning to the Lucas-Washburn regime.

maybe use this eq instead of shorted one?

$$\pi r^2 \rho l \frac{du}{dt} = 2\pi r \gamma \cos \theta_a + \pi r^2 \rho g h - 8\pi \mu l u - \frac{3}{2} \pi r^2 \rho u^2 - 2\pi r \gamma \cos \theta_a f \quad (2.16)$$

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## 2.3 Simulating the Wetting Processes

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Simulating a two-phase flow can be achieved through several methods. Common approaches include the Volume-of-Fluid and the Level-Set methods. Both methods use a sharp interface and are based on the Hydrodynamic Theory from Chapter 2.2.1. Moreover, they are *interface capturing* methods, so they don't require recalculating the computational grid over the simulation period. Other methods that follow the interface (*interface tracking*) are also possible. One of the major drawbacks of these methods is that the moving contact line, when using the adhesion condition, depends on models [9].

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Additionally, calculating the surface tension can pose a challenge. This requires computing the curvature of the surface, which can lead to relatively high numerical errors [27, 21].

The Lattice-Boltzmann Method uses collision models to describe fluid behavior. Surface tensions can be considered through modifications. There are approaches that are promising and some are comparable to the phase-field method. However, one of the biggest challenges is the limitation of density or viscosity ratios. In this work, the fluids have significantly different densities with a ratio of 1000. According to [10], the Lattice-Boltzmann Method is limited to ratios of  $\mathcal{O}(10)$  and can lead to instabilities otherwise.

Another frequently used method is **Molecular Dynamic** simulations. Since individual molecules are simulated in this case, this method is only applicable to geometrically and temporally small problems without driving computational costs too high. Therefore, **Molecular Dynamic** simulations are often used for comparison or to study only small problems ([13, 29, 31, 15]).

The method used in this work is the **phase-field** method. This method models two or even multi-phase flow through the system's free energy. A more detailed description of this method and the simulations already carried out is provided in Chapter 3.

Elaborate or maybe move the entire section to phase field? Or perhaps case setup with a reasoning why phase field?



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## 3 Phase Field Method

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The phase field method, rooted in system thermodynamics, offers a solution for an interface with a finite thickness, an idea originating from van der Waals in 1893 [38]. This method models the free energy of the system and can derive a phase field method for interfacial dynamics. It offers several advantages, such as mass conservation, contact line motion, and adherence to thermodynamic laws. In contrast to the hydrodynamic theory, the contact line moves through interfacial diffusion. However, there are concerns about its validity in modeling macroscopic contact line motion, especially regarding the sharp-interface limit. Despite these concerns, meaningful results have been predicted on the macro scale that align with hydrodynamic theory and experimental observations[44, 42, 8].

Phase field simulations for macroscopic wetting typically rely on the Cahn-Hilliard equations. For slow wetting phenomena, the phase field theory has been both analytically [26] and numerically [42, 44] proven to capture such wetting physics. However, for rapid spreading of water drops, the assumption of local equilibrium may not hold. Some studies have introduced a boundary condition for wetting far from equilibrium, introducing a parameter that controls the relaxation towards equilibrium. This parameter has been interpreted in various ways, from a local friction adjacent to the contact line to a relaxation parameter at the contact line[43][9].

**Phase Field Theory** Die Phasenfeld theorie verwendet Ansätze beider Modelle unter verwendung der Beschreibung der freien Energie des Systems.

Daher ist es auch notwendig für die Phasenfeldmethode sowohl hydrodynamische Ansätze als auch Ansätze der Molekular Kinetik Theorie zu verwenden [3, 9].

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Free energy system

einleitende Worte

Wie bereits in Kapitel 2.1 beshrieben, gibt es unterschiedliche Möglichkeiten das Interface zu beschreiben. Hydrodynamische Modelle beschreiben das Interface so, dass am Übergang der Phasen die Stoffwerte springen. Ein Diffuses Interface hingegen, beschreibt die großen anders.

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## 3.1 Phase Field Method in the Spirit of Cahn and Hillard

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The phase field method traces back to the idea of van der Waals [38], who described the interface between two immiscible fluids from a thermodynamic perspective. In this description, the material properties transition continuously within a thin layer. Within this layer, both phases coexist.

Building on this, Cahn and Hillard [28] derived a description of the free energy in a volume with non-uniform composition as a function of an order parameter  $C$  for time-dependent problems. In its closed form, it reads

$$\partial C + \mathbf{u} \cdot \nabla C = \nabla \cdot (\kappa \nabla \phi(C)). \quad (3.1)$$

Here,  $\mathbf{u}$  is the velocity,  $\kappa$  is a diffusion coefficient, often referred to as mobility, and  $\phi$  is a chemical potential. The order parameter indicates which phase is present and ranges between  $-1$  and  $1$  for a two-phase system. The mobility can be related to the Péclet number, which represents the ratio of advective to diffusive fluxes with a characteristic path length ( $L_{char}$ ) and velocity ( $u_{char}$ ), as well as a characteristic chemical potential [7, 23].

The chemical potential is defined as the derivative of the Helmholtz free energy with respect to the order parameter [28]. In the system under consideration, the total free energy consists of the mixing energy and the interfacial density energy. According to [44], the system's free energy is influenced by two factors; defined over the volume  $\Omega$  and the surface  $\partial\Omega$

$$F(C, \nabla C) = \int_{\Omega} f_{\text{mix}}(C, \nabla C) d\mathbf{x} + \int_{\partial\Omega} f_w(C) dS \quad (3.2)$$

Here, the first integral represents the mixing energy density  $f_{\text{mix}}$ , and the second represents the wall energy  $f_w$ .

### 3.1.1 Mixing Energy

Cahn and Hillard defined a mixing energy ( $f_{\text{mix}}$ ) that depends on the order parameter and its gradient:

$$F(C, \nabla C) = \int_{\Omega} f_{\text{mix}}(C, \nabla C) d\mathbf{x} = \int_{\Omega} \left( \frac{\lambda}{\epsilon^2} \Psi(C) + \frac{\lambda}{2} |\nabla C|^2 \right) d\mathbf{x} \quad (3.3)$$

The integration of the mixing energy over the domain yields the Helmholtz free energy of the fluid system and consists of two terms. The first term separates the phases from each other, while the second term mixes the phases.  $\lambda$  is a mixing energy parameter,  $\epsilon$  a measure for the thickness of the interface, and  $\Psi$  a potential. The potential is chosen according to Ginzburg and Landau so that it has two minima at positions  $-1$  and  $1$  and is

check!!!

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check if already mentioned

cite

given by

$$\Psi(C) = \frac{1}{4} (C^2 - 1)^2. \quad (3.4)$$

This leads to the following representation for the chemical potential

$$\Phi(C) := \frac{\partial F(C)}{\partial C} = \frac{\lambda}{\epsilon^2} \Psi'(C) - \lambda \nabla^2 C. \quad (3.5)$$

### 3.1.2 Diffusive Interface

The Cahn-Hilliard model can describe systems with multiple fluids. However, only a binary fluid system is considered in this work. Figure 3.1 shows the contact line of a

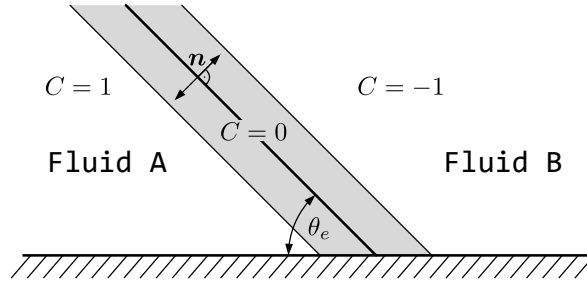


Figure 3.1: Schematic representation of a diffusive interface

diffusive interface. The gray area is the transition area of the order parameter and thus the material quantities. Within this area, both fluids coexist with their respective densities and viscosities. In the equilibrium state, the profile of  $C$  normal to the interface can be determined by minimizing the free energy (Equation 3.5) [7]. This then leads to a description of the order parameter normal to the interface with

$$C(n) = \tanh \left( \frac{n}{\sqrt{2}\epsilon} \right). \quad (3.6)$$

Here,  $n$  is the normal to the interface. In equilibrium, the thickness of the diffuse interface remains constant in a range of  $3/\sqrt{2}\epsilon$  and for the order parameter  $-0.9 \leq C \leq 0.9$ . Also in the case of equilibrium, the surface tension equals the integral of the free energy density at the interface, from which a description for the surface tension can be derived [26].

$$\sigma = \int_{-\infty}^{\infty} \lambda \left( \frac{dC}{dn} \right)^2 = \frac{2\sqrt{2}}{3} \frac{\lambda}{\epsilon} \quad (3.7)$$

### 3.1.3 Wall Energy

Jacqmin [25] postulated a wall energy of the form

$$F_w = \int \sigma g(C) dA, \quad (3.8)$$

where the wall energy is now only a function dependent on the fluid composition directly at the wall. The resulting natural phase field boundary condition with local thermal equilibrium is given by

$$\lambda \frac{\partial C}{\partial n_{\partial\Omega}} + f'_w(C) = 0. \quad (3.9)$$

With  $n_{\partial\Omega}$  as the normal direction on the wall (cf. 3.1). The normal direction to the interface can be described with the wall normal and wall tangential direction on the wall.

$$n = n_{\partial\Omega} \cos(\theta_e) + \tau_{\partial\Omega} \sin(\theta_e). \quad (3.10)$$

Subsequently, for the first term from Equation 3.9 with Equations 3.10, 3.6, and 3.7, the following can be established

$$\lambda \frac{\partial C}{\partial n_{\partial\Omega}} = \underbrace{\frac{3}{4} \sigma (1 - C^2) \cos \theta_e}_{=:-f'_w(C)}. \quad (3.11)$$

From this, a function for the wall energy density can be derived after integration [26][23].

$$f_w(C) = -\sigma \cos \theta_e \frac{C(3 - C^2)}{4} + \frac{\sigma_{S_L} + \sigma_{S_V}}{2} \quad (3.12)$$

When only one of the phases is present, this equation only returns the respective surface tension. However, Yue et al. [43] point out that this description of wall energy for equilibrium contact angles close to  $0^\circ$  or  $180^\circ$  is difficult to reproduce, and the model is not capable of handling precursor films.

**Non Equilibrium Boundary Condition** In aller Regel wird die Gleichgewichts Randbedingung verwendet (Gleichung 3.9) und vernachlässigen dabei ungleichgewichte nahe der Wand. Jacqmin [26] entwickelte und Yue et al. [43] bzw. Qian et al. [33] studierten eine generalisierte Variante von Gleichung 3.9.

$$\frac{\partial C}{\partial t} + \mathbf{u}_w \cdot \nabla C = -\Gamma_w \underbrace{\left( \lambda \frac{\partial C}{\partial n_{\partial\Omega}} + f'_{w(C)} \right)}_{=:\phi_w} \quad (3.13)$$

Mit  $\Gamma_w$  als einer neu eingeführten Konstante, genannt *wall relaxation parameter*. Die Geschwindigkeit der Wand ist durch  $\mathbf{u}_w$  gegeben. Nach Qian et al. [33] folgt für  $\Gamma_w \rightarrow 0$

und  $\kappa \rightarrow 0$  das sharp interface limit mit dominanter advektion. Für den gegenteiligen Fall folgt eine dominante Diffusion. Der wall relaxation parameter ist ein parameter ist für die Simulation eine Einstellgröße und sollte as phänomenologischer parameter verstanden werden. Dieser parameter hängt sowohl vom Fluid system als auch von der Fluid wand Kombination ab[26].

## 3.2 Cahn-Hillard Navier Stokes Equations

The coupled Cahn-Hillard Navier Stokes equations are given by

$$\partial_t C + \nabla \cdot (C\mathbf{u}) = -\nabla \cdot \mathbf{J} \quad (3.14)$$

$$\nabla \cdot \mathbf{u} = 0 \quad (3.15)$$

$$\partial_t(\rho\mathbf{u}) + \nabla \cdot (\rho\mathbf{u}\mathbf{u}) = -\nabla\tilde{p} + \nabla\tau - \nabla \cdot (\mathbf{u}\mathbf{J}) - \phi\nabla C + \mathbf{f}_b \quad (3.16)$$

Wherein,  $\tilde{p}$  is a modified pressure that arises from the Korteweg tensor to account for capillarity. Assuming a Newtonian fluid,  $\tau = 2\mu\text{dev}\mathbf{D}$  with  $\mathbf{D} = 1/2[\nabla\mathbf{u} + (\nabla\mathbf{u})^T]$  as the deformation tensor. Furthermore, the density  $\rho$  and viscosity  $\mu$  are volumetrically averaged with

$$\rho = \frac{1+C}{2}\rho_1 + \frac{1-C}{2}\rho_2. \quad (3.17)$$

Here, the suffixes 1 and 2 are markers for the respective phases. The viscosity is calculated analogously. The term  $-\nabla \cdot (\mathbf{u}\mathbf{J})$  is necessary to ensure thermal consistency [16].  $\mathbf{J}$  is the phase-field flux and, according to Landau and Lifshitz,  $\mathbf{J} = -M\nabla\phi$ .

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### 3.2.1 Boundary Conditions

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## 4 Case Setup

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Die Geometrie und einige Stoffeigenschaften sind durch die in 2 definierten vereinfachungen und Annahmen bereits vorgegeben. Im folgen wird zu beginn die Geometrie der Kapillare vorgestellt, gefolgt von den Materialeigenschaften und verwendeter Randbedingungen. Da mehrere Untersuchungen unternommen wurden, erfolgt in Kapitel eine Übersicht über die durchgeführten Simulationen und dessen Initialisierung.

Wie bereits in Kapitel 1 geschrieben, erfolgen die Simulationen mit dem solver `phaseFieldFoam`. Dieser wurde bereits mehrfach Validiert, worauf in Kapitel 5 genauer eingegangen wird.

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### 4.1 Geometry

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Die Geometrie der Kapillare wird so angenommen, dass sie wie in Abbildung 4.1 zu sehen ein Reservoir mit Wasser hat, welches durch Oberflächeneffekte in die Kapillare strömt. Durch die Annahme, dass sich ein Teil des Wassers bereits in der Kapillare befindet, wird in der Simulieren Geometrie lediglich die Randbedingung so gesetzt, dass das Wasser in diesem Reservoir nachströmen kann. Die Dimensionen der Kapillare ergeben sich daraus, dass die Simulation der Kapillare perspektivisch auch mit experimenten verglichen werden soll. Daher wurden auch weitere, komplexere Geometrien simuliert, die jedoch nicht Teil dieser Arbeit sind. Wie zu erkennen, handelt es sich um eine Kapillare mit lediglich  $6\text{nm}$  Durchmesser. Eine Simulation so kleiner Kapillare wurde soweit bekannt bisher nicht mit der Phasenfeld methode Simuliert.

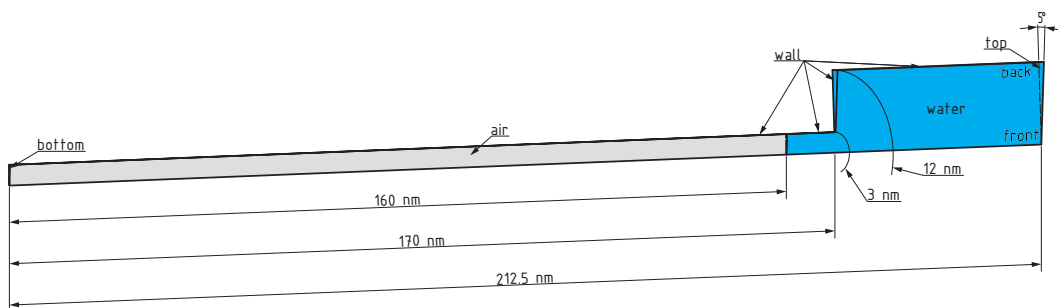


Figure 4.1: Schematic of used Capillary

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Die Diskretisierung der Geometrie wurde so gewählt, dass die Elemente eine Kantenlänge von  $0.2nm$  haben. In Radialer Richtung hat eine Wedge nur ein Element.

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## 4.2 Randbedingungen

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In Abbildung 4.1 sind neben der Geometrie auch die Flächen, die mit Randbedingungen versehen wurden benannt. Die Flächen `front` und `back` sind sich gegenüberliegende Flächen der Wedge und müssen dementsprechende Randbedingungen erhalten. Die `wall` Flächen sind nicht durchdringbare Oberflächen und `top`, bzw. `bottom` Oberflächen durch die ein Fluss zugelassen wird. Im folgenden werden die Randbedingungen für die Oberflächen für die unterschiedlich durchgeführten Simulationen einzeln gezeigt.

**wall** wie ebenfalls schon erwähnt werden sowohl Simulationen mit als auch ohne die Gleichgewichtsrandbedingung durchgeführt. Generell sind die Randbedingungen für beide Fälle gleich. An einer Stelle unterscheiden sie sich jedoch voneinander. Im Falle der Gleichgewichtsrandbedingung gelten für die Wand die folgenden Randbedingungen

Table 4.1: relevant boundary conditions wall

Parameter	Value
orderparameter $C$	<code>equilibriumPhaseContactAngle</code>
equilibrium contact angle $\theta_e$	<code>15°, 45°, 75°</code>
chemisches Potential $\phi$	<code>zeroGradient</code>
velocity $\mathbf{u}$	<code><math>\mathbf{u}_w = 0</math></code>
pressure $p$	<code>fixedFluxPressure</code>

Für den Ordnungsparameter  $C$  wird die Gleichgewichtsrandbedingung angenommen und der Gleichgewichtskontaktwinkel für jede der drei Simulationen mit dieser Geometrie mit  $15^\circ$ ,  $45^\circ$  bzw.  $75^\circ$  angegeben. Der Gradient des chemischen Potentials an der Wand wird als null gesetzt, genauso wie die Geschwindigkeit der Wand. Die Randbedingung für den Druck wird mit `fixedFluxPressure` so gewählt, dass der Druckgradient so angepasst wird, dass der Massenfluss am Rand mit der vorgegebenen Geschwindigkeit an der Wand übereinstimmt.

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## 5 Validation

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The phaseFieldFoam- Solver

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## 6 Results

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The Position of the meniskus was exported with paraview in the decomposed state. The position was then extracted with a python script. Probe data was preprocessed as well and several computations for eval of simulations. Plots were generated with matplotlib?; Start of real results with an overview when what where. Maybe work with normalized data?



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## 7 Outlook

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- complex geometry
- temperature dependent capillary rise?
- surfactants and capillary rise?
- more fluids with other viscosities

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