# Modeling of the Boundary Regions between a Spreading Droplet and a Rough Surface of Solid

T. Theis, A. Ouazzi, O. Mierka, S. Turek

*Chair of Applied Mathematics & Numerics (LS3), Department of Mathematics*

## Abstract

Drop impact onto a solid surface is a complex phenomenon, which is depending on a variety of factors. To describe the fluid motion, the incompressible Navier-Stokes equations will be used. It is known that the inertial effects and the viscous and surface tension forces affect the evolution of the drop spreading and accordingly of the receding. The arising singularity in the solution for the stresses at the contact line requires special treatment. The interface is divided into three regions with different length scales. At the inner region, the local viscous drag near the moving contact line determines the value of the microscopic dynamic contact angle. Due to numerical difficulties to resolve a mesh of the order of the slip length, which is comparable with the molecular size, the inner region is removed from the computational domain. We substitute the interplay between the microscopic angle and the macroscopic hydrodynamics by an additional force applied to the contact line. The Navier slip boundary conditions appear on the intermediate region. At the outer region the inertial effects become significant. This region is characterized by the no-slip boundary condition. Both fluids are assumed to be incompressible and Newtonian with constant properties (density, viscosity and surface tension). Some preliminary numerical results for an axisymmetric problem are presented.

***Keywords:*** *Contact line speed, macroscopic and microscopic dynamic contact angle, slip length, drop spreading, Navier-Stokes equations*

## 1 Motivation

In collaboration with the Chair of Computer Science VII, the robot-guided thermal spray process will be simulated on different levels. The micro- and macroscopic characteristics of the layer are the key aspects of the project. For the prediction of the coating thickness the understanding of the interaction between droplets and substrate is essential. The drop impact onto a rough solid surface is a widely studied problem. This study has focused on the drop deformation and its spreading on the wall. The classical approach for laminar incompressible two-phase flow is described by the Navier-Stokes equations:

$$\rho_i(u_t + u \cdot \nabla u) - \nabla \cdot (\mu_i(\nabla u + \nabla u^T) + \nabla p = \rho_i g + f$$
$$\nabla \cdot u = 0$$

in which the density $\rho_i$ and viscosity $\mu_i$ are variable and discontinuous, $i \in \{1,2\}$. The shear stress tensor will be denoted with $S_i = \mu_i(\nabla u + \nabla u^T)$. The moving interface $\Gamma$ of the droplet is unknown and must be determined in every time step. The well-known Level Set approach represents the interface as zero isoline of a continuous distance function $\phi$:

$$\phi(x,t) = \begin{cases} dist(x,\Gamma), & \forall\, x \in liquid\ 1 \\ -dist(x,\Gamma), & \forall x \in liquid\ 2\ (the\ droplet) \end{cases}$$

An overview how to use Level Set techniques is given in [Tur12]. When the position of the interface between two liquids is known, the boundary conditions will be defined as follows:

- The normal velocity at the interface in both liquids shall be identical with the interface motion
- The continuity of tangential velocity
- The continuity of tangential stress: $(S_1 - S_2) \cdot \tau_{1,2} = 0$
- The balance of the normal stress on the interface:

  $(S_1 - S_2) \cdot n_{1,2} = \sigma \kappa n_{l1,2}$

The boundary conditions between the viscous fluid and the rough solid will be specified as follows: The traditional no-slip condition predicts that an infinite force is required to move the contact line. This is the so-called “contact-line problem”, referring to the non-integrable singularity in the shear stress. This stress singularity is avoided by replacing the no-slip condition by the Navier slip condition for the velocity component along the wall. However, for the major part of the drop the permitting slip is not valid [Fer12]. For macro-scale flow the interaction between the Newtonian fluid and the wall is equivalent to the no-slip boundary condition. Hence, several regions with different length scales will be considered. In the immediate vicinity of the contact line the slip effect is significant. The slip length is a measure of the extent of this region. For an accurate resolution of the flow, the mesh size should be less than the slip length. Unfortunately [Sik05] this length is not observed in experiments because it is much smaller than the size corresponding to one pixel on the drop image. Therefore, the slip length is much smaller than the mesh size in the numerical simulations. So that it cannot be calculated. To circumvent this problem, the inner region is removed from the computational domain and replaced by a compensative force $f_{cl}$, applied to the moving contact line. Due to the continuity of the velocity field it is not favorable to calculate the drop with the no-slip condition and an additional force at the contact line. An intermediate region is needed as well [Cox86]. There is a small region near the interface, where the Navier slip condition is valid.

To prescribe the "contact-line" force $f_{cl} = \sigma \cos \theta_w$, the specification of the microscopic dynamic contact angle $\theta_w$ is required. This is the angle between the interface and the solid surface at the contact line. The microscopic contact angle $\theta_w$ plays a significant role in the dynamics. The value of $\theta_w$ is assumed to be a function of the static (equilibrium) contact angle $\theta_e$ and the capillary number $Ca = \frac{\mu V_{cl}}{\sigma}$, where $V_{cl}$ is the velocity of propagation of the contact line. The velocity of the contact line $V_{cl}$ is not a material velocity. An accurate estimation of the velocity $V_{cl}$ influences the modeling problem.

Examples of the so-called "contact line problem", which can be experimentally investigated and as well numerically computed, occur with

- The spreading of a liquid drop on a horizontal surface
- The movement of a drop down an inclined surface
- The movement of a solid object through a liquid interface
- The inkjet printing
- The coating process

## 2 Mathematical Model

As mentioned before, the boundary between the droplet and the solid surface will be separated into three regions. At the outer region the traditional no-slip boundary condition is valid. The Reynolds number based on the drop size is considerable and the inertia effect is not negligible. The macroscopic dynamic contact angle $\theta_a$ can be predicted from the drop shape in the numerical simulation. This angle is called the apparent dynamic contact angle. It is shown in **Fig. 1** and can be determined experimentally.

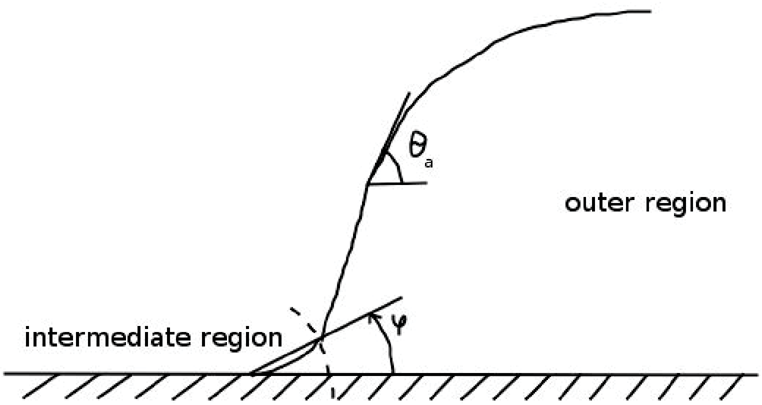


***Fig. 1:*** *Outer region of the droplet size length scale;* $\boldsymbol{\theta_a}$ *represents the macroscopic (apparent) dynamic contact angle.*

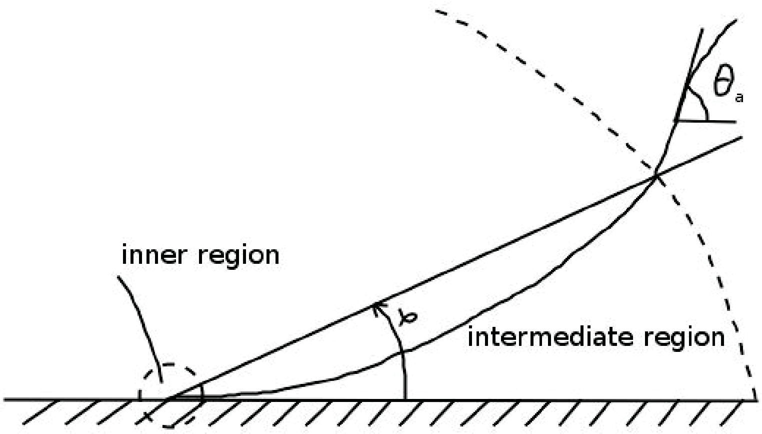


***Fig. 2:*** *Intermediate region of the size of* $\boldsymbol{O(1/|\ln\beta|)}$*, where the slip effect is significant and* $\boldsymbol{\beta}$ *is the slip length.*

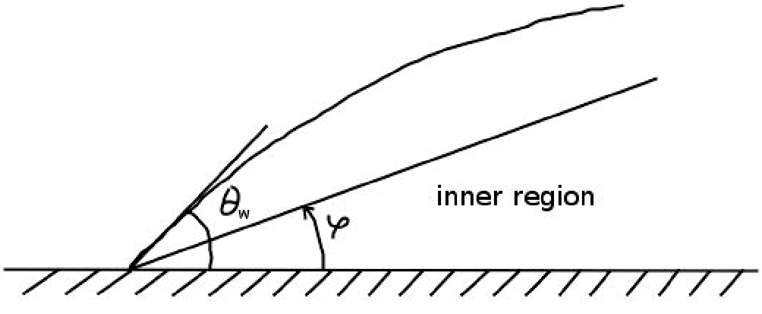


***Fig. 3:*** *Inner region in the vicinity of the moving contact line;* $\boldsymbol{\theta_w}$ *represents the microscopic (wetting) dynamic contact angle.*

The intermediate region is a region, where the influence of the acceleration $dV_{cl}/dt$ becomes significant. Slip between the liquid and the solid occurs very close to the contact line (**Fig. 2**). The Reynolds number based on the slip length is very small and the flow is dominated by viscous forces. The Navier slip boundary condition will be used. The most popular slip model [Fer12] relates the slip velocity to the wall velocity gradient via the proportionality coefficient:

$$u_{ws} = \beta \frac{du}{dy}$$

where the coefficient $\beta$ is named slip length. The slip velocity along the wall is denoted with $u_{ws}$. The size of this region is of the order of $O(1/|\ln \beta|)$ [Sui13].

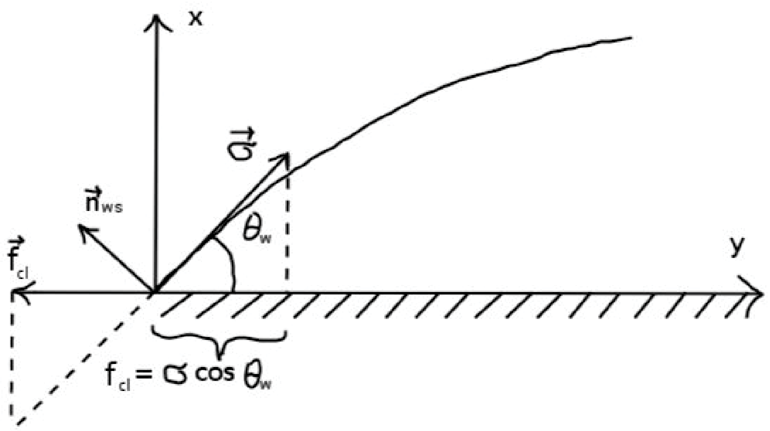


***Fig. 4:*** *Contact-line force, according to Young's equation.*

The contact-line force $f_{cl} = \sigma \cos \theta_w$, applied parallel to the wall, substitutes the inner region. **Figure 4** illustrates this definition. The force is related to the viscous drag and capillary effects in the corner. The microscopic dynamic contact angle $\theta_w$ is shown in **Fig. 3, 4** and assumed to be a function of the static contact angle $\theta_e$ and the capillary number [Sui13], [Sik05], [Cox86].

## 3 Numerical Results

The first numerical test concerns an axisymmetric droplet. The simulation considers only one half of the droplet. The full droplet simulations yield exactly symmetric results. The solid surface is idealized as being perfectly flat, smooth, dry, and chemically homogeneous. A simpler model of the contact-line force was proposed, in which the velocity of propagation of the contact line is assumed to be a constant.

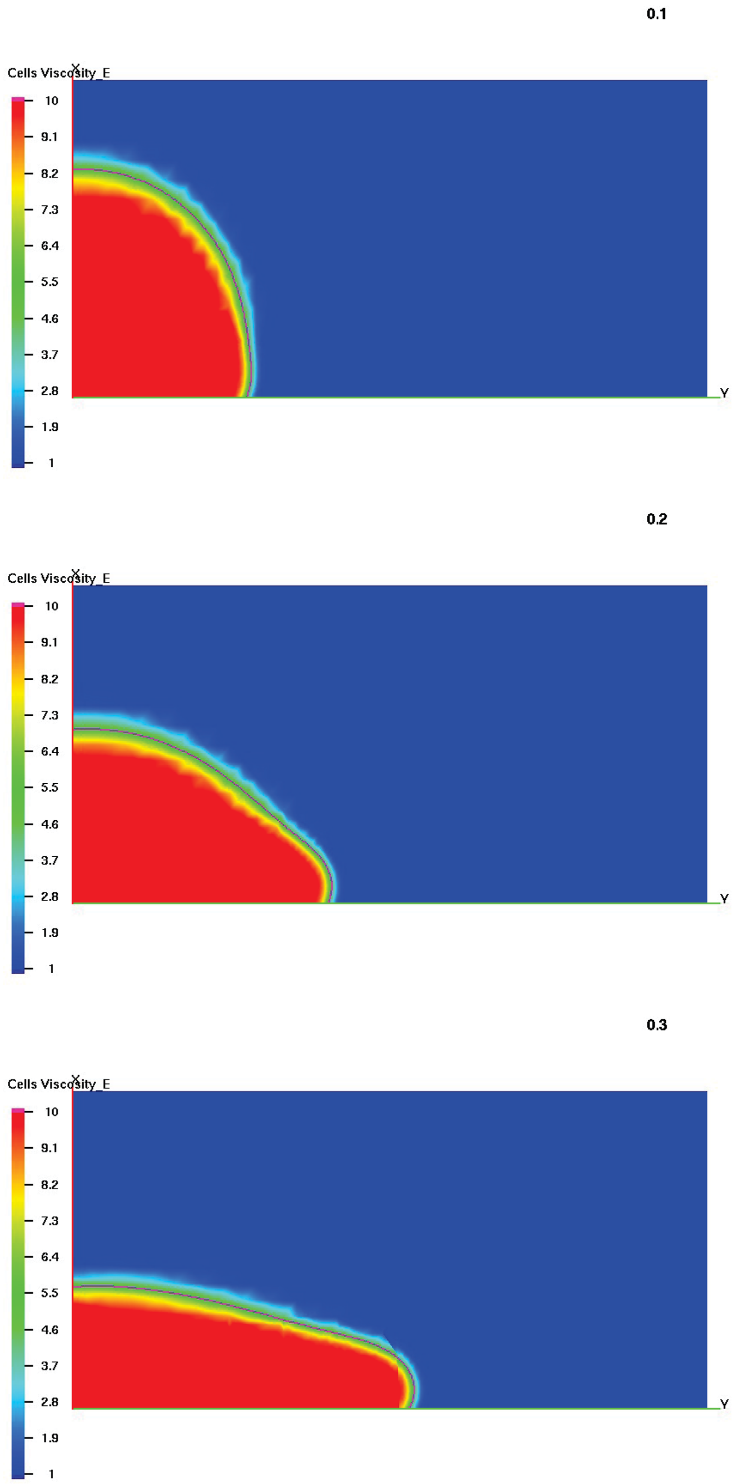


***Fig. 5:*** *Qualitative comparison of the drop shape at several time instants.*

The parameters of the presented simulations are given in in **Tab. 1**. The model is shown to converge and agree with previous work.

*Tab. 1: The parameters of the simulations.*

| **Characteristics** | **Length scale** | **Liquid 1** | **Liquid 2 (Drop)** |
|---|---|---|---|
| Contact - line vel. $V_{cl} = 15.5\ \frac{m}{s}$ | Droplet size $R = 2.5\,mm$ | Viscosity $\mu_1 = 1\ \ \mu Pa \cdot s$ | Viscosity $\mu_2 = 10\ \ \mu Pa \cdot s$ |
| Static cont. angle $\theta_e = \ 75^{\circ}$ | Slip length $\beta = 10^{-8}\ mm$ | Density $\rho_1 = 10^5\ \frac{kg}{m^3}$ | Density $\rho_2 = 10^6\ \frac{kg}{m^3}$ |
| Gravity constant $g = -9.8\ \frac{m}{s^2}$ | Domain size $5\ \times 10\,mm$ | Surface tension $\sigma = 250\ \frac{N}{m}$ | |

In this example, we demonstrate that in order to include the drop impact some mechanisms are necessary to predict the moving contact line. Then, one needs first to prescribe the contact-line force and the contact-line speed for the boundary condition between the droplet and the substrate. The grid should be refined to such an extent, that the intermediate region can be resolved. Any mesh of size larger than $1/|\ln\beta|$ will lead to mesh size dependent results.

## 4 Conclusion

The modeling of the drop spreading on a flat surface with the effect of the microscopic contact line is formulated and currently numerically tested. The preliminary results from the present model show a qualitative agreement with the physical expectation. The comparison of the numerical results with the experiment is under ongoing work.

## 5 Acknowledgement

The authors gratefully acknowledge the financial support of the DFG (German Research Foundation) within the Collaborative Research Centre SFB 708, project B1, and the LiDOng cluster at the TU Dortmund.

## References

[Tur12] Turek, S.; Mierka, O.; Hysing, S.; Kuzmin, D.: Numerical study of a high order 3D FEM-Level Set approach for immiscible flow simulation. Repin, S., Tiihonen, T., Tuovinen, T., Computational Methods in Applied Sciences, Vol. 27, 65-70, Numerical methods for differential equations, optimization, and technological problems, Springer, ISBN 978-94-007-5287-0, (2012)

[Cox86] Cox, R. G.: The Dynamics of the Spreading of Liquids on a Solid Surface. Part 1. Viscous Flow. Journal of Fluid Mechanics, 168 (1986), p. 169-194

[Sik05] Sikalo, S.; Wilhelm, H.-D.; Roisman, I. V.; Jakirlic, S.; Tropea C.: Dynamic Contact Angle of Spreading Droplets: Experiments and Simulations. Physics of Fluids, 17 (2005), p. 062103:1-13

[Sui13] Sui, Y.; Spelt, P. D. M.: An Efficient Computational Model for Macroscale Simulations of Moving Contact Lines. Journal of Computational Physics, 242 (2013), p. 37-52

[Fer12] Ferras, L. L.; Nobrega, J. M.; Pinho, F. T.: Analytical Solutions for Newtonian and Inelastic Non-Newtonian Flows with Wall Slip. Journal of Non-Newtonian Fluid Mechanics, 175-176 (2012), p. 76-88