Simulation of Wash-off Processes on Inclined Surfaces

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Introduction

Motivation:
To simulate industrial processes like spray cooling of surfaces [1], coating or wash off processes, e.g. during a reactor accident, modeling of dynamic wetting is an essential requirement. Understanding the formation, breakdown and the dynamic behavior of mainly gravity driven rivulets is crucial to simulate and predict wash-off processes.

Objectives: Development of a CFD model to describe the dynamics of rivulets and thin liquid films

- Simulate thin water films and their transition into rivulets
- Find the key influencing quantities of the transition process
- Investigate the stability of rivulets and partially wetting films in time and space
- Characterize paths of the rivulets and the spatial dry/wet distribution
- Calibrate and validate the model

Mathematical Modeling

The one-fluid formulation of isothermal, incompressible, variable-density Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad (1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \mathbf{I} - \mu \mathbf{S} - \rho \mathbf{g} - \sigma \mathbf{n} \kappa \delta_S) = 0 \qquad (2)$$

describes the dynamics of multiphase flows where $\mathbf{S} = \nabla \mathbf{u} + \nabla^T \mathbf{u}$ is the deformation rate. The curvature of the surface κ is defined by

$$\kappa = -\nabla \cdot \left(\frac{\nabla \alpha}{|\nabla \alpha|} \right). \qquad (3)$$

The phase interface is captured by a Volume-of-Fluid (VOF) method. A scalar volume fraction field α, the indicator function which represents the fractional volume of fluid within one cell and ranges from 0 to 1, is tracked by the transport equation with an additional compression term to sharpen the liquid gas interface

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u} \alpha) = 0. \qquad (4)$$

Contact Angle

The most determining region in wash-off processes is the dynamic wetting line. Here the moving liquid interface seems to intersect with the solid beneath it at a visible contact angle. The contact angle between surface, fluid and gas has huge impact on the behavior of a gravity driven water film, such as the transition into rivulets and droplets.

Effects on several scales ranging from molecular scale (wall layer) to macroscopic scale (velocity of the flow field) play a role in dynamic wetting. One can distinguish between the macroscopic scale, which corresponds to the contact angle used in the simulations, the microscopic scale and the molecular scale, where there is no sharp wetting line but a wetting region and hence the concept of a single contact angle fails.

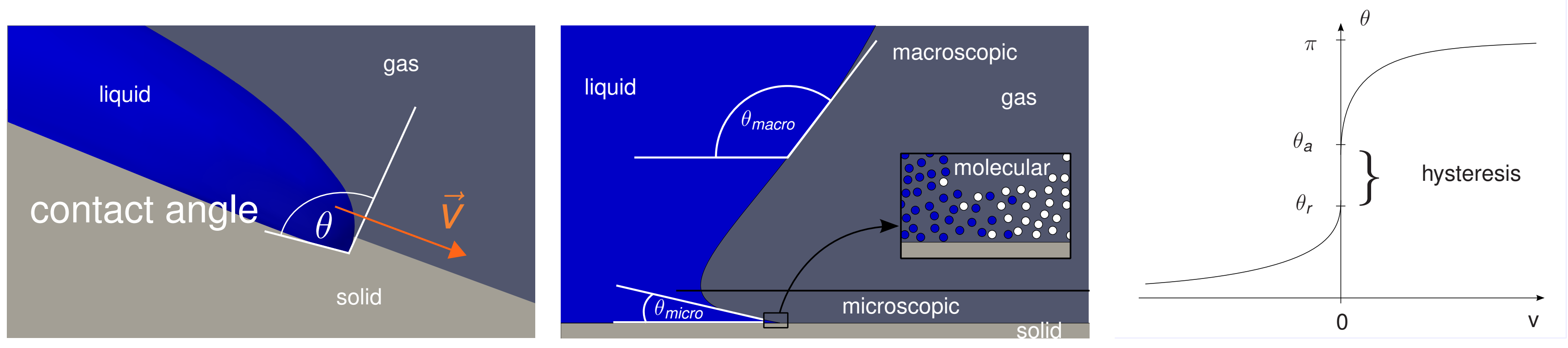

Figure 1 : Contact angle at different scales: macroscopic scale (left), microscopic scale and molecular scale with symbolic blue water and white air molecules (middle) and contact angle hysteresis andvelocity dependency (right).

The Kistler model [2] for the so called dynamic contact angle takes into account the velocity dependency: θ_D rises with contact line velocity and $\theta_D = \theta$ if $\vec{v} = 0$ with θ being the equilibrium contact angle.

$$\theta_D = f_h(Ca + f_h^{-1}(\theta)), \quad f_h(x) = \arccos\left(1 - 2\tanh(5.12 \left(\tfrac{x}{1+1.31x^{0.99}}\right)^{0.706}\right) \qquad (5)$$

with $Ca = \frac{\mu v}{\sigma}$ the capillary number. It holds: $\lim_{v\to\infty} \theta_D = \pi$ and $\lim_{v\to 0} \theta_D = \theta$.

Dynamic wetting systems often exhibit contact angle hysteresis [3]: the advancing contact angle θ_a is the largest contact angle at which the contact line still is at rest but is at the egde of moving from wet to dry surface. It differs from the receding contact angle θ_r, the smallest contact angle that occurs right before the contact line moves from dry to wet surface, cf. Fig. 1 right.

Simulation Setup

The simulation domain is a three-dimensional trapezoid plate according to the experiments by [4], with a rectangular zone at the upper most end to avoid errors arising from initial and boundary conditions at the inlet.

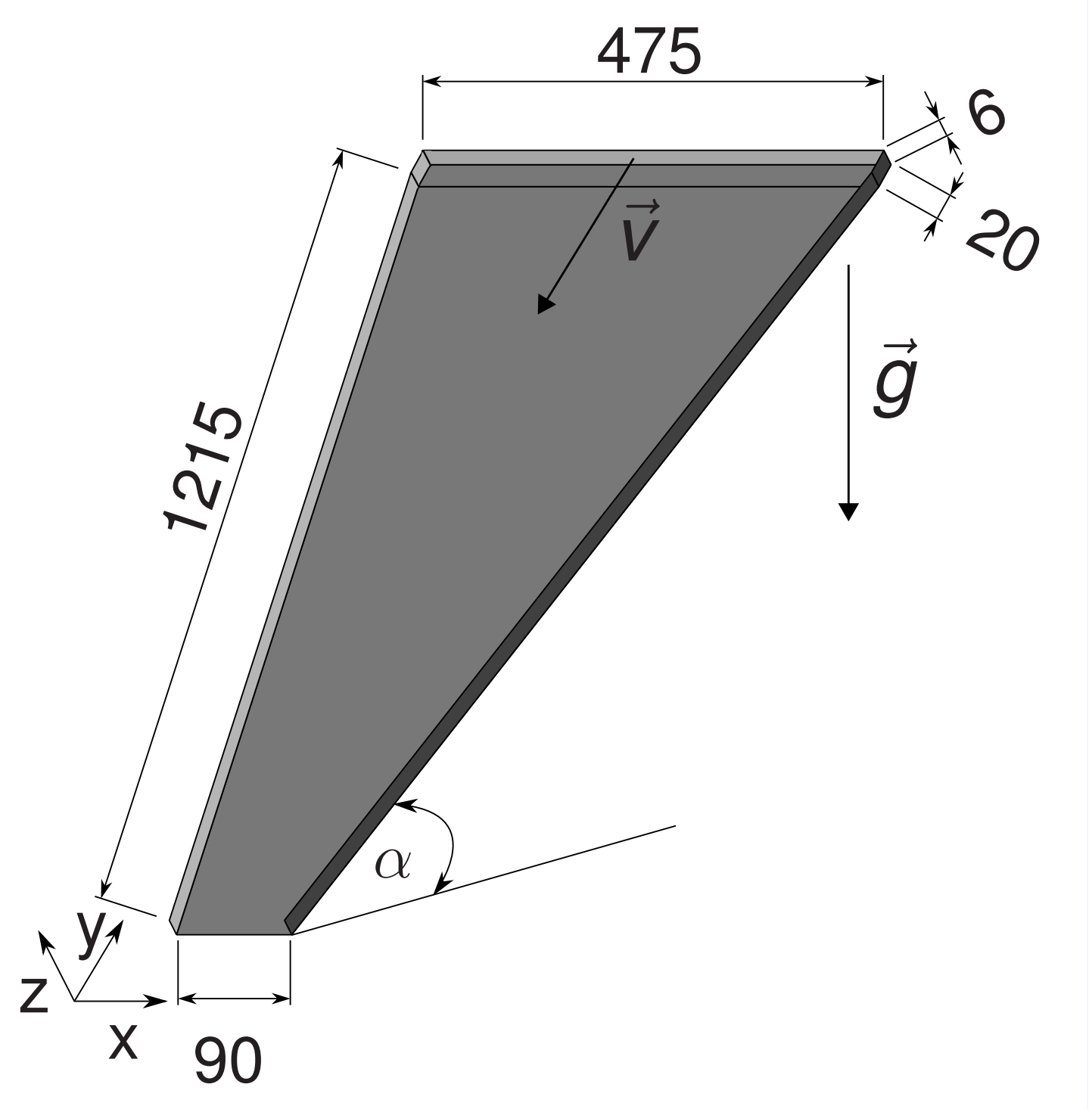

Figure 2 : Simulation domain: trapezoid plate with rectangular inlet region, side walls and inclination angle α, all dimensions are in [mm].

Initially the plate is dry. At the inlet water enters the computational domain with a velocity parallel to the plate such that a given mass flow rate is achieved. At the floor and the side walls a no slip boundary condition holds. The plate is tilted by the inclination angle α. The structured grid is refined near walls. No turbulence model is needed due to laminar flow.

Results

Within the simulations the influence of the inclination angle α, the mass flow rate, the contact angle model and the contact angle value(s) are investigated. The results of the simulations are described in terms of pattern formation. The behavior can be characterized by comparing and identifying the water height, the fraction of wetted and dry surface area and the mean run-down velocity.

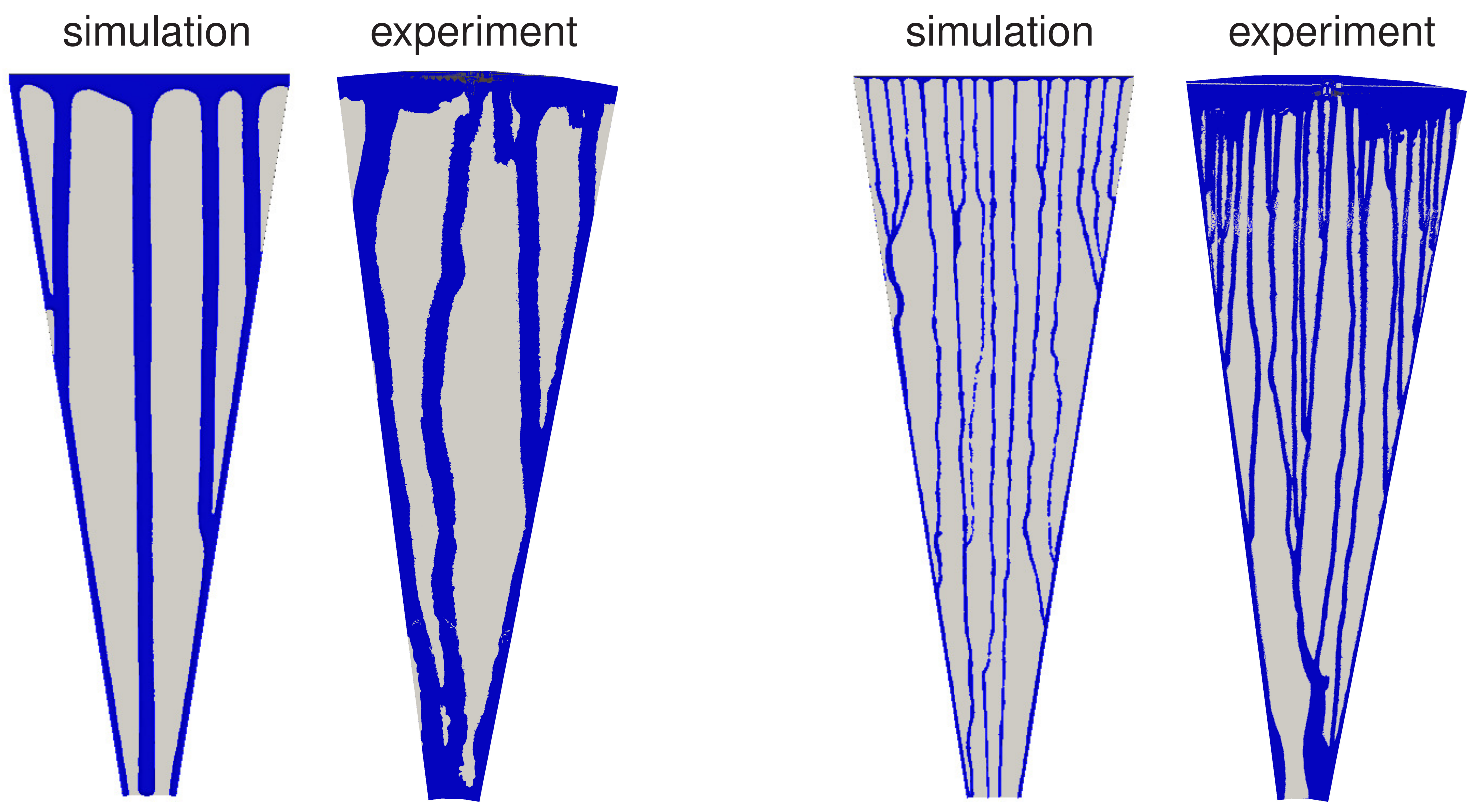

Figure 3 : Topview of the plate with inclination angle 2° (a) and 20° (b). Different rivulet number and width for different inclinations. Simulations left and experiments [4] (false colour representation) right, respectively.

A first result can be seen in Fig. 3, where the run down behavior of the water clearly changes with the inclination angle: $\alpha_{3a} = 2^\circ$ and $\alpha_{3b} = 20^\circ$. The contact angle is constant and accounts for the wetted history ($\theta_{dry} = 100^\circ$, $\theta_{wet} = 15^\circ$) and the mass flow rate is 11g/s. The same behaviour is observed in the experiments [4] with the same inclination and mass flow rate (see Fig. 3a and 3b on the right).

Outlook

- Include sediment transport approaches
- Check stability and behavior of rivulets on inhomogeneous surfaces
- Consider effects of vapor condensation
- Develop a (semi-empirical) model

References

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[4] von Laufenberg, B., Colombet, M., Freitag, M. (2014). Wash-down of insoluble aerosols. Result of the Laboratory Tests related to THAI AW3 Test, unpublished manuscript.