New perspectives on capillary rise from complexity reduced models

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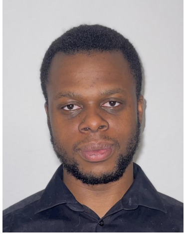
CRC 1194 Interaction between Transport and Wetting Processes

Mathematical Modeling and Analysis

Acknowledgements: Thanks to all my co-workers!

(a) M. Fricke

(b) S. Raju

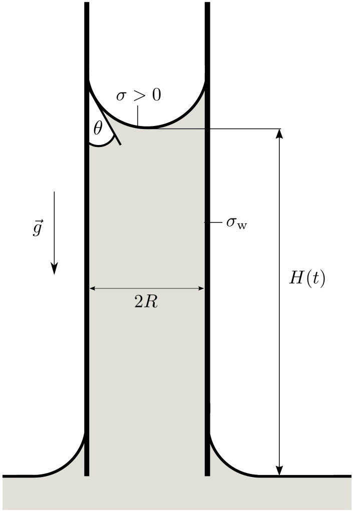


(c) E. A. Ouro-Koura

(d) J. De Coninck

(e) D. Bothe

Capillary rise: A prototypical (dynamic) wetting process



- **Free energy** functional (including some approximations):

$$\mathcal{E}(h) = \pi R^2 \sigma + 2\pi R h \sigma_w + \frac{\pi}{2} \rho g R^2 h^2.$$

  σ_w: specific energy due to **wetting** of the solid

- Young equation for the equilibrium **contact angle**

$$\sigma \cos\theta_0 + \sigma_w = 0.$$

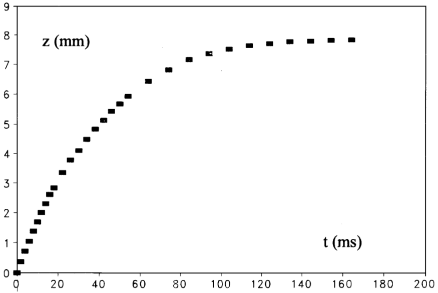
- Energy **minimization** yields Jurin's equation

$$h_0 = -\frac{2\sigma_w}{\rho g R} = \frac{2\sigma\cos\theta_0}{\rho g R}$$

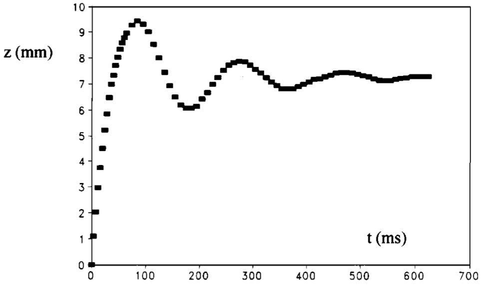
  describing the stationary rise height.

Dynamics of capillary rise

- There are different **regimes** for the rise **dynamics** observed in experiments.
- (Quéré, Europhys. Lett., 1997):
  Monotone rise for ethanol, **oscillatory** rise for ether (low viscosity).
- **Goal: Predict** the dynamics from material parameters. This is (still) a challenging problem!



(a) Ethanol ($\eta = 1.17$mPa $\cdot$ s).

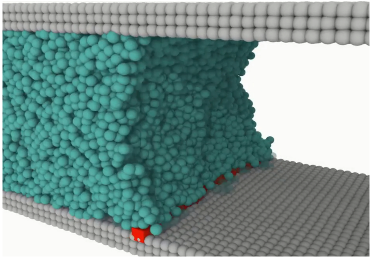


(b) Ether ($\eta = 0.3$mPa $\cdot$ s).

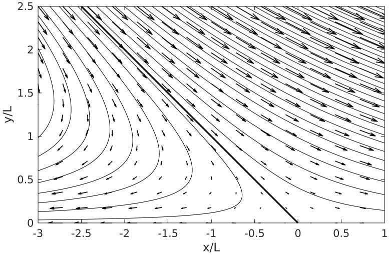
Figure: Experimental data by Quéré (1997). Capillary rise in a glass tube ($R = 0.689$mm).

A hierarchy of models for dynamic wetting

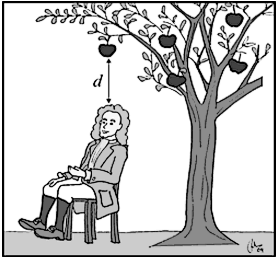
- **Molecular dynamics:** Accurate description of the local physics. Limited to short length and time scales.
- **Continuum mechanics:** Small scale physics "encoded" in constitutive laws and boundary conditions.
- **Simplified models:** Models derived from continuum mechanics using some simplifying approximations. Here: Aim for **ordinary differential equations**.



(a) Molecular dynamics.



(b) Continuum mechanics.



(c) Simplified models.

Figure (c) taken from www.aps.org/publications/apsnews/200908/zerogravity.cfm.

Outline

1. Direct numerical simulations of capillary rise dynamics
2. Complexity-reduced models and rise height oscillations
3. Summary and Outlook

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A numerical benchmark for dynamic wetting simulations

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A comparative study of transient capillary rise using direct numerical simulations

Check for updates

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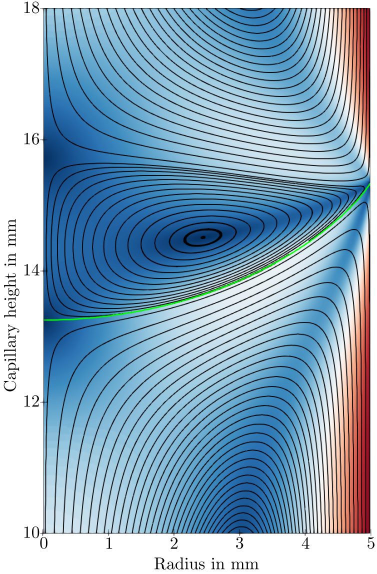
- Gründing et al.: *A comparative study of transient capillary rise using direct numerical simulations* [Grü+20a]

A numerical benchmark for dynamic wetting simulations



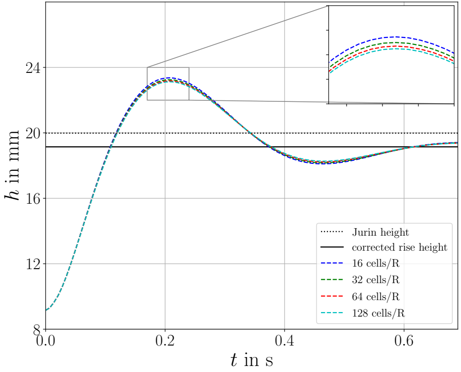
- **Observation:** There is a lack of accurate **reference** solutions.
- **Goal:** Establish a **numerical benchmark** for an instationary dynamic wetting problem.
- **Mathematical model:** Sharp interface two-phase Navier Stokes equations with fixed contact angle and Navier slip condition

$$-v_{||} = 2L(Dn)_{||} \quad \text{at } \partial\Omega.$$

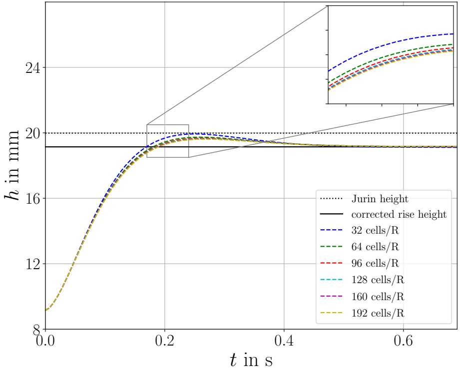
- We provide an **extensive dataset** [Grü+20b] validated with **four different** numerical methods.

Influence of the slip length

- **Finding:** The slip length may change the character of the rise dynamics.



(a) $L = R/5$.



(b) $L = R/50$.

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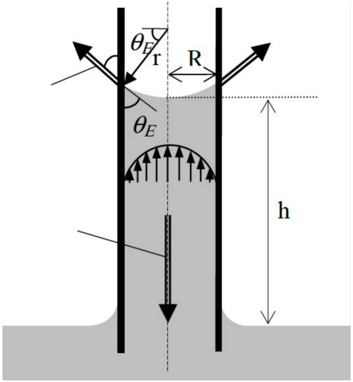
The classical model by Bosanquet



- **Classical model** due to Bosanquet (1923):

$$\boxed{2\pi R\sigma\cos\theta_0 = 8\pi\eta h\dot{h} + \frac{d}{dt}(\pi R^2 h\rho\dot{h}) + \pi R^2 h\rho g.} \qquad (1)$$

"Capillary force = Viscous resistance + inertia + gravity"

- **Simplifying assumptions:** Flat interface Σ (to compute M), Poiseuille flow profile (with no slip condition).

$$\text{Volume: } V = \pi R^2 h, \quad \text{Mass: } M = \rho V,$$

$$\text{Momentum: } P = M\dot{h}.$$

- Only **one** dissipative process modeled:
Viscous dissipation in the **Poiseuille flow** region.

Non-dimensional form

- Using the length and time scales

$$h_0 = \frac{2\sigma \cos\theta_0}{\rho g R} \quad \text{and} \quad t_{\text{ref}} = \sqrt{h_0/g}$$

in (1), one arrives at

$$\boxed{1 = (HH')' + \Omega\, HH' + H.} \tag{2}$$

- Here $H(\tau) = h(\tau t_{\text{ref}})/h_0$ is the dimensionless rise height. The **dimensionless group**

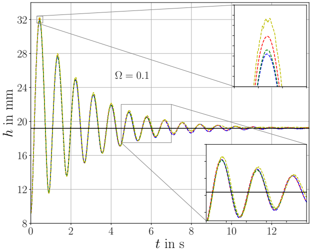
$$\boxed{\Omega = \sqrt{\frac{128\eta^2\sigma\cos\theta_0}{R^5\rho^3 g^2}} = \sqrt{128\cos\theta_0}\,\frac{\text{Oh}}{\text{Bo}}}$$

governs the behaviour of solutions of (2).

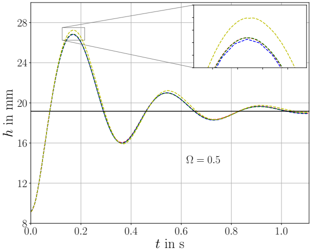
- Quéré showed that a **regime transition** for (2) occurs at

$$\Omega_c = 2.$$

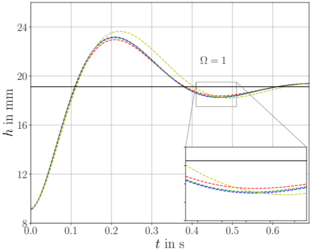
Variation of the parameter Ω in the DNS



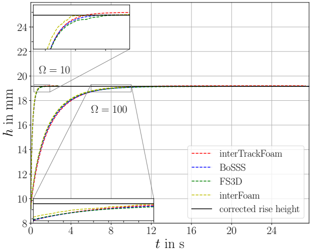
(a) $\Omega = 0.1$



(b) $\Omega = 0.5$



(c) $\Omega = 1$



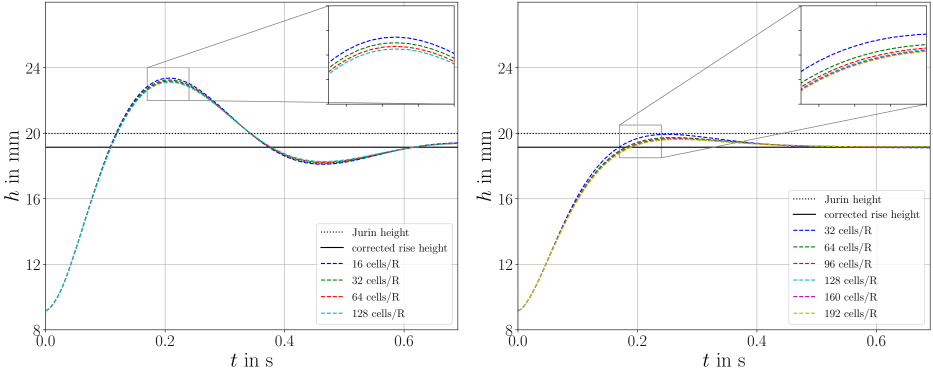
(d) $\Omega = 10, 100$

Guiding research question

- Can we derive a **generalization** of Quere's critical condition?

$$\Omega = \sqrt{\frac{128\eta^2\sigma\cos\theta_0}{R^5\rho^3 g^2}} < 2$$

- The parameter Ω does **not involve** the slip length! **A dissipative process is missing in the model!**



(a) $L = R/5$.　(b) $L = R/50$.

Capillary rise with dynamic contact angle effect

- **Dynamic contact angle model:** The Molecular Kinetic Theory yields (as Ca $\to 0$)

$$\sigma \left(\cos\theta_0 - \cos\theta\right) = \zeta V_\Gamma \tag{3}$$

with a friction coefficient $\zeta \geq 0$. This leads to a quadratic term for the **contact line dissipation**

$$\sigma \int_{\Gamma(t)} \left(\cos\theta - \cos\theta_0\right) V_\Gamma \, dl = -\zeta \int_{\Gamma(t)} V_\Gamma^2 \, dl \leq 0.$$

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- The resulting model reads as (see Martic et al., Langmuir, 2002 [Mar+02])

$$\frac{2}{R}\sigma\cos\theta_{eq} = \frac{8\eta}{R^2}h\dot{h} + \rho\frac{d}{dt}(h\dot{h}) + \rho g h + \frac{2}{R}\zeta\dot{h}. \tag{4}$$

$\Rightarrow$ Dissipation **at the contact line** is added to the classical model.

- The new term $\propto \dot{h}$ has a different **mathematical structure**.

$\Rightarrow$ A **second non-dimensional parameter** is introduced into the problem.

Capillary rise with dynamic contact angle effect

- Experimental data by Quéré [Qué97] (open circles) are well described.
- **Best fit for the friction:** $\zeta = 80\,\text{mPa}\cdot\text{s}$.
- **Regime transition** is observed: (a) $\zeta = 80\,\text{mPa}\cdot\text{s}$, (b) $\zeta = 0$.
- **Question:** What is the critical condition for this model?

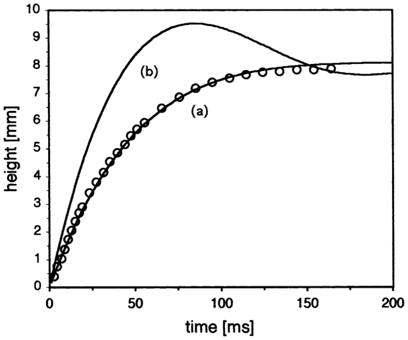


Figure: Results for ethanol from (Martic et al.,2003).

Critical condition for "Martic type" models

- We study models of the general form

$$(HH')' + \Omega\, HH' + \beta H' + H = 1. \tag{5}$$

- The parameter β may originate from different physical mechanisms. For example, in Martic's model, we have

$$\beta = \frac{\zeta}{\sqrt{\sigma \rho R \cos\theta_0}}.$$

- We show[1] that the generalization of the critical condition reads as

$$\boxed{\Omega + \beta < 2.} \tag{6}$$

- Hence, the oscillatory regime is **shifted** towards smaller values of Ω for positive β.

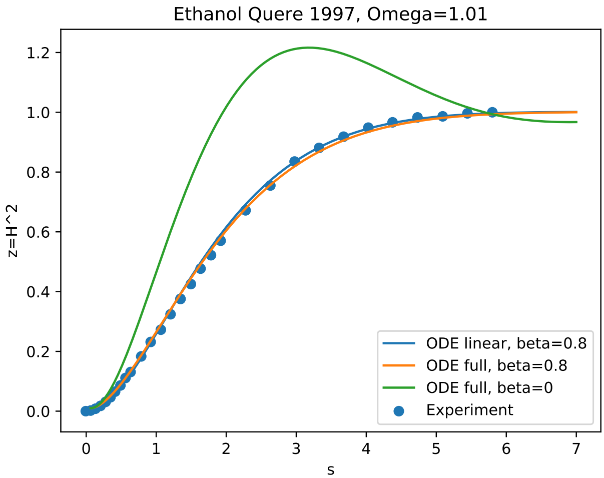
[1] This part is joint work with El Assad Ouro-Koura (B. Sc.). His Bachelor Thesis on the topic has the title "Zur mathematischen Modellierung des kapillaren Anstiegs: Dissipative Mechanismen und nicht-lineare Oszillationen", TU Darmstadt (2023).

Comparison with experimental data (I)

- Using the fit from Martic et al. for the data for ethanol by Quere, we have

$$\beta = \frac{\zeta}{\sqrt{\sigma \rho R \cos \theta_0}} \approx \frac{80\,\mathrm{mPa \cdot s}}{107\,\mathrm{mPa \cdot s}} \approx 0.75, \quad \Omega \approx 1.01.$$

- We expect **oscillations** since $\Omega + \beta \approx 1.8 < 2$ (!).



Comparison with experimental data (II)

- In fact, the **analytical theory** gives more information than just the critical damping condition.

[2] For details, we refer to our upcoming preprint.

Comparison with experimental data (II)

- In fact, the **analytical theory** gives more information than just the critical damping condition.
- From a linearization of the problem, we obtain[2]

$$H(s)^2 \approx 1 + \exp\left(-\frac{\Omega + \beta}{2} s\right) A \cos(\omega s + \phi), \tag{7}$$

where $\omega = \sqrt{1 - (\Omega + \beta)^2 / 4}$.

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Comparison with experimental data (II)

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where $\omega = \sqrt{1-(\Omega+\beta)^2/4}$.

- Note that the dimensionless time-period of oscillation

$$S = \frac{2\pi}{\sqrt{1-(\Omega+\beta)^2/4}} \to \infty \quad \text{as} \quad \Omega+\beta \to 2$$

goes to infinity as the critical damping is approached. The **exponential decay part** will dominate in this case.

- In the present example, we have

$$S = \frac{2\pi}{\sqrt{1-1.8^2/4}} \approx 14.4.$$

[2]For details, we refer to our upcoming preprint.

Comparison with experimental data (III)

- **Idea:** We can visualize the **oscillatory part** of the solution (7) by factoring out the exponential decay. Hence, we plot the function

$$\Psi(s) := \exp\left(\frac{\Omega+\beta}{2}\, s\right)\left(H(s)^2 - 1\right).$$

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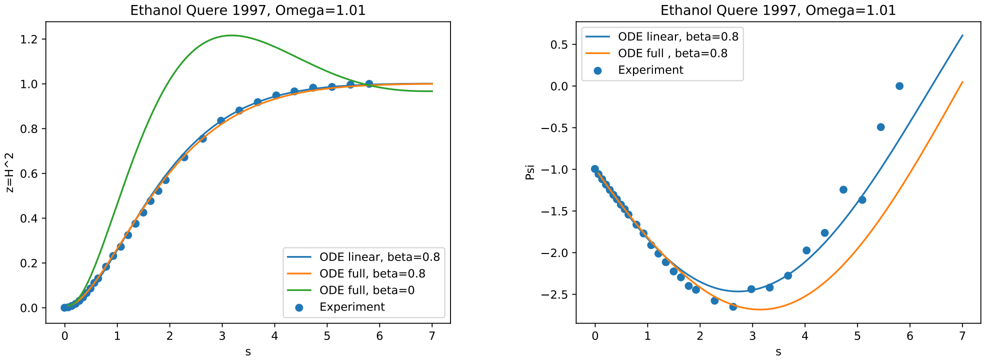
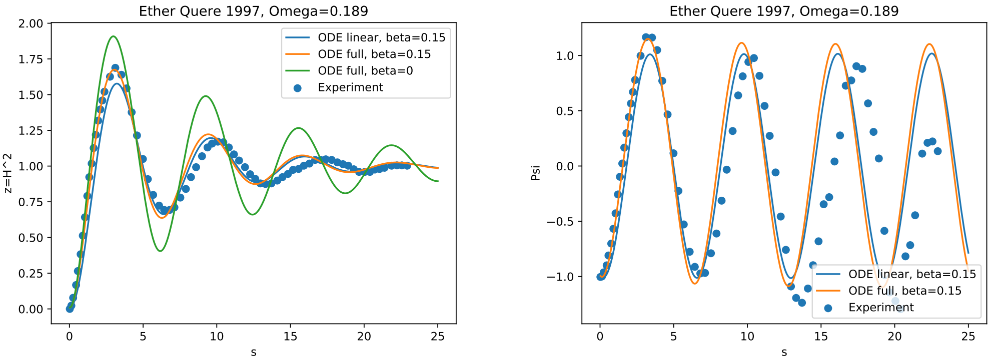


- Indeed, the oscillation is **confirmed** from the experimental data.

Comparison with experimental data (IV)

- The model is also able to describe the strong oscillations of **ether** in [Qué97] quite well. In this case, the system is far from critical damping.

$$\Omega \approx 0.19, \quad \beta \approx 0.15 \quad \Rightarrow \Omega + \beta \approx 0.34 < 2.$$



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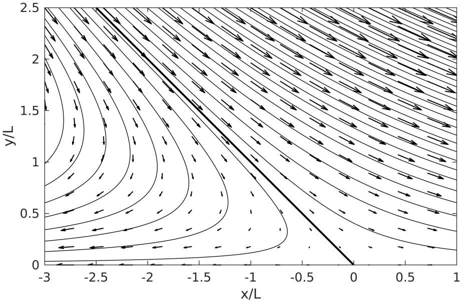
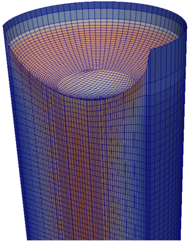
Including dissipation near the contact line: The model by Gründing

- D. Gründing: *An enhanced model for the capillary rise problem* (IJMF, 2020) [Grü20]
- **Major contribution:** Modeling of viscous dissipation in the **contact line vicinity**.
  $\Rightarrow$ Effect of the **slip length** on the dissipation can be modeled.
- Known **asymptotic solutions** are used ($\Delta^2\psi = 0$, stream function ψ).
- Has the **same mathematical structure** like the model by Martic et al.

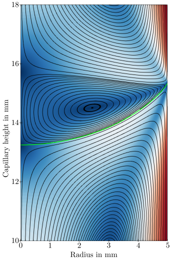


Summary and Outlook

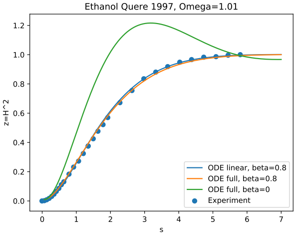
- Derivation of **complexity-reduced (ODE) models** guided by DNS.
- **Framework** for ODE models: Variational formulation using different **channels of dissipation** (to be modeled from DNS)[3].
- Mathematical analysis of ODE leads to new **physical insights**.
- In Progress: **Calibration** of ODE models with DNS to make predictions **beyond** current DNS capabilities.
- **Long-term goal:** Subgrid-scale models for the moving contact line?



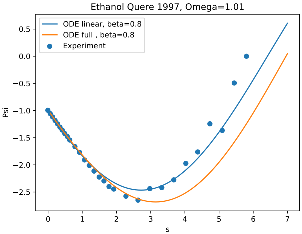
(a) DNS.



(b) Local flow.



(c) ODE model.



(d) Oscillation.

[3]Please check out our upcoming preprint for more details.

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References I

[BC02] T.D Blake and J De Coninck. “The influence of solid–liquid interactions on dynamic wetting”. In: *Advances in Colloid and Interface Science* 96.1-3 (Feb. 2002), pp. 21–36. DOI: 10.1016/s0001-8686(01)00073-2.

[BH69] T.D Blake and J.M. Haynes. “Kinetics of liquid-liquid displacement”. In: *Journal of Colloid and Interface Science* 30.3 (July 1969), pp. 421–423. ISSN: 00219797. DOI: 10.1016/0021-9797(69)90411-1.

[Bos23] C. H. Bosanquet. “On the flow of liquids into capillary tubes”. In: *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* 45.267 (Mar. 1923), pp. 525–531. ISSN: 1941-5982. DOI: 10.1080/14786442308634144.

[Grü+20a] D. Gründing et al. “A comparative study of transient capillary rise using direct numerical simulations”. In: *Applied Mathematical Modelling* 86 (May 2020), pp. 142–165. ISSN: 0307904X. DOI: 10.1016/j.apm.2020.04.020.

[Grü+20b] D. Gründing et al. *A comparative study of transient capillary rise using direct numerical simulations: Benchmark Data*. 2020. DOI: 10.25534/tudatalib-173.

[Grü20] D. Gründing. “An enhanced model for the capillary rise problem”. In: *International Journal of Multiphase Flow* (Jan. 2020), p. 103210. ISSN: 03019322. DOI: 10.1016/j.ijmultiphaseflow.2020.103210.

References II

[Mar+02] G. Martic et al. "A Molecular Dynamics Simulation of Capillary Imbibition". In: *Langmuir* 18.21 (Sept. 2002), pp. 7971–7976. DOI: 10.1021/la020068n.

[MCB03] G. Martic, J. De Coninck, and T.D. Blake. "Influence of the dynamic contact angle on the characterization of porous media". In: *Journal of Colloid and Interface Science* 263.1 (July 2003), pp. 213–216. DOI: 10.1016/s0021-9797(03)00283-2.

[Qué97] D. Quéré. "Inertial capillarity". In: *Europhysics Letters (EPL)* 39.5 (Sept. 1997), pp. 533–538. DOI: 10.1209/epl/i1997-00389-2.