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Dynamic wetting of cellulosic substrates by model liquids

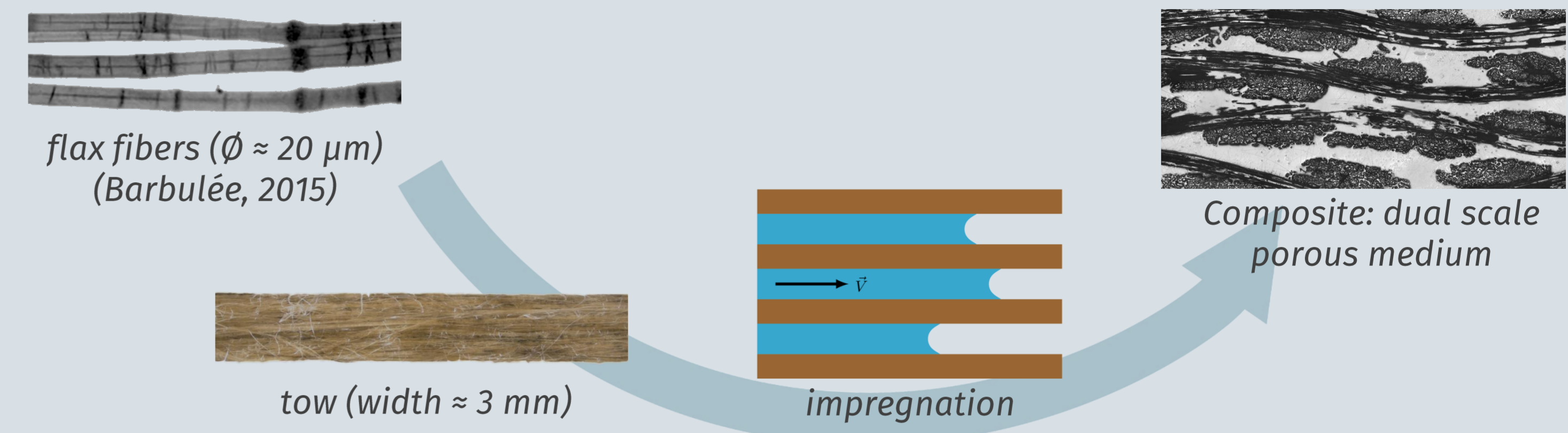
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Motivation

The processing of **flax-polymer composites** is a **multiscale** problem, requiring an accurate description of **capillary flows** occurring inside and between the tows. Since natural fibers exhibit complex structure, **model materials** are used to implement the processing mechanisms. The main goals are:

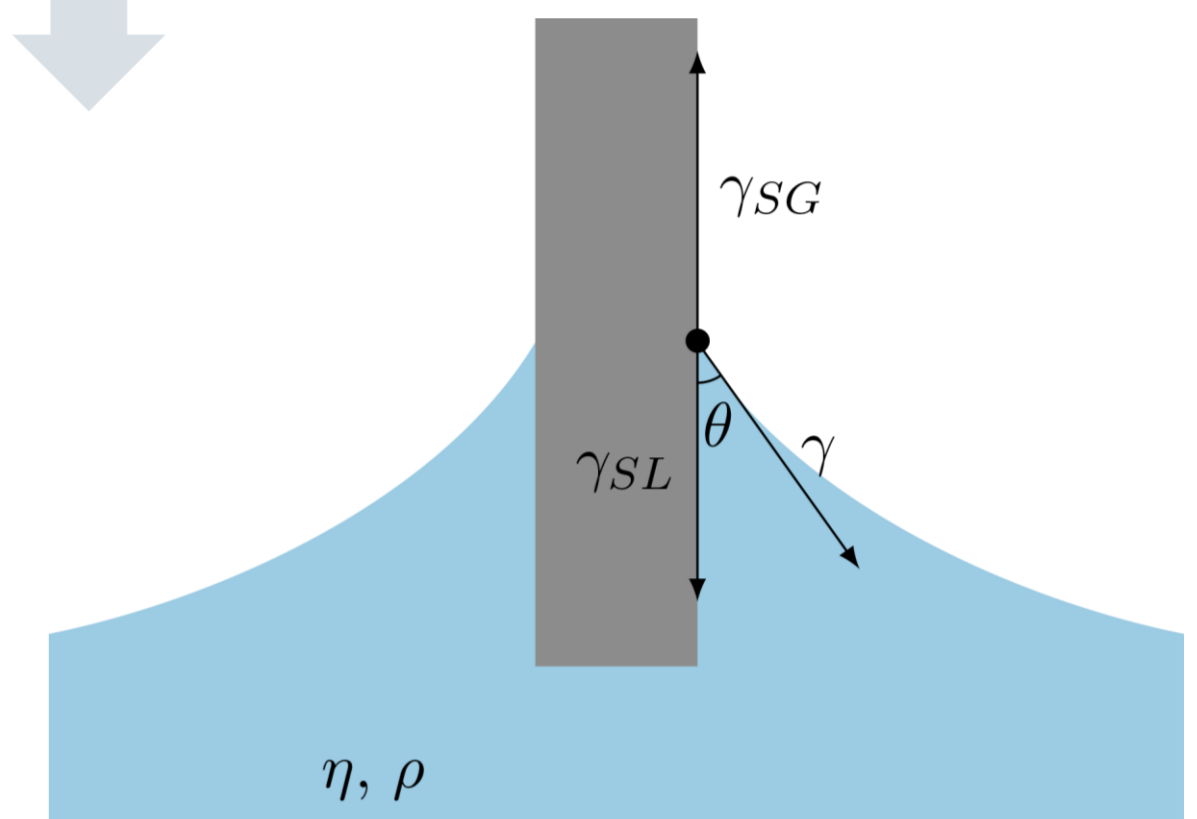
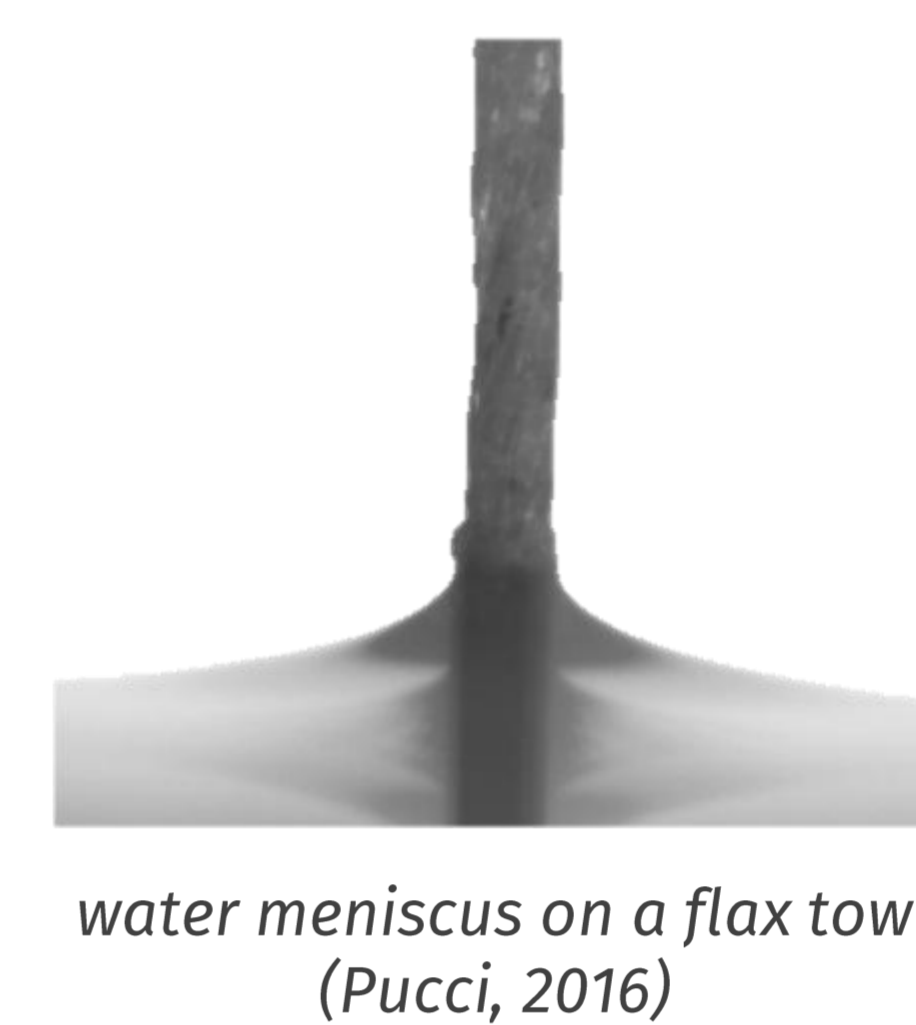
- modeling dynamic wetting phenomena for cellulose-polymer systems
- assessing the influence of physical parameters on dynamic wetting regimes
- evaluating the accuracy of existing models



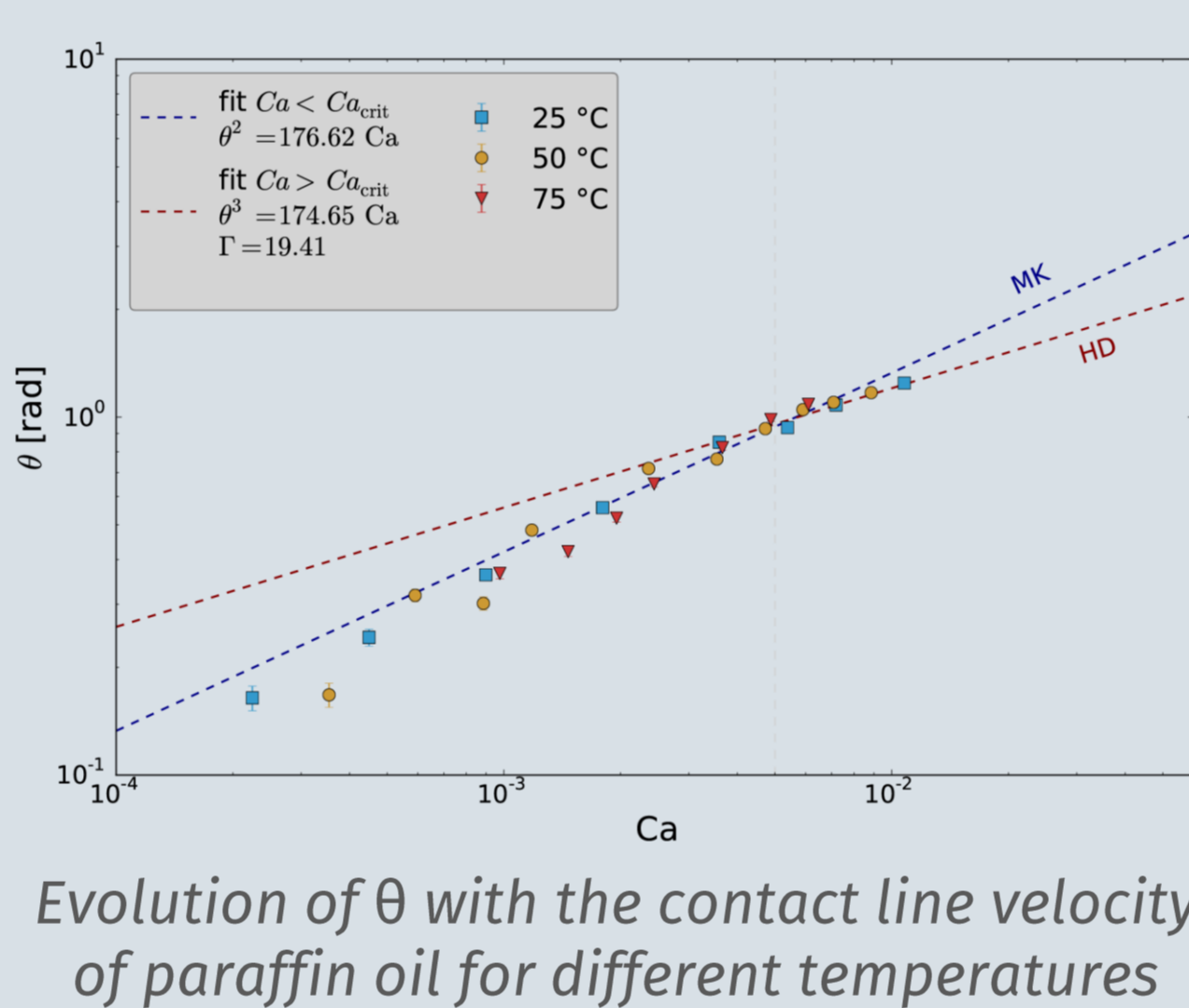
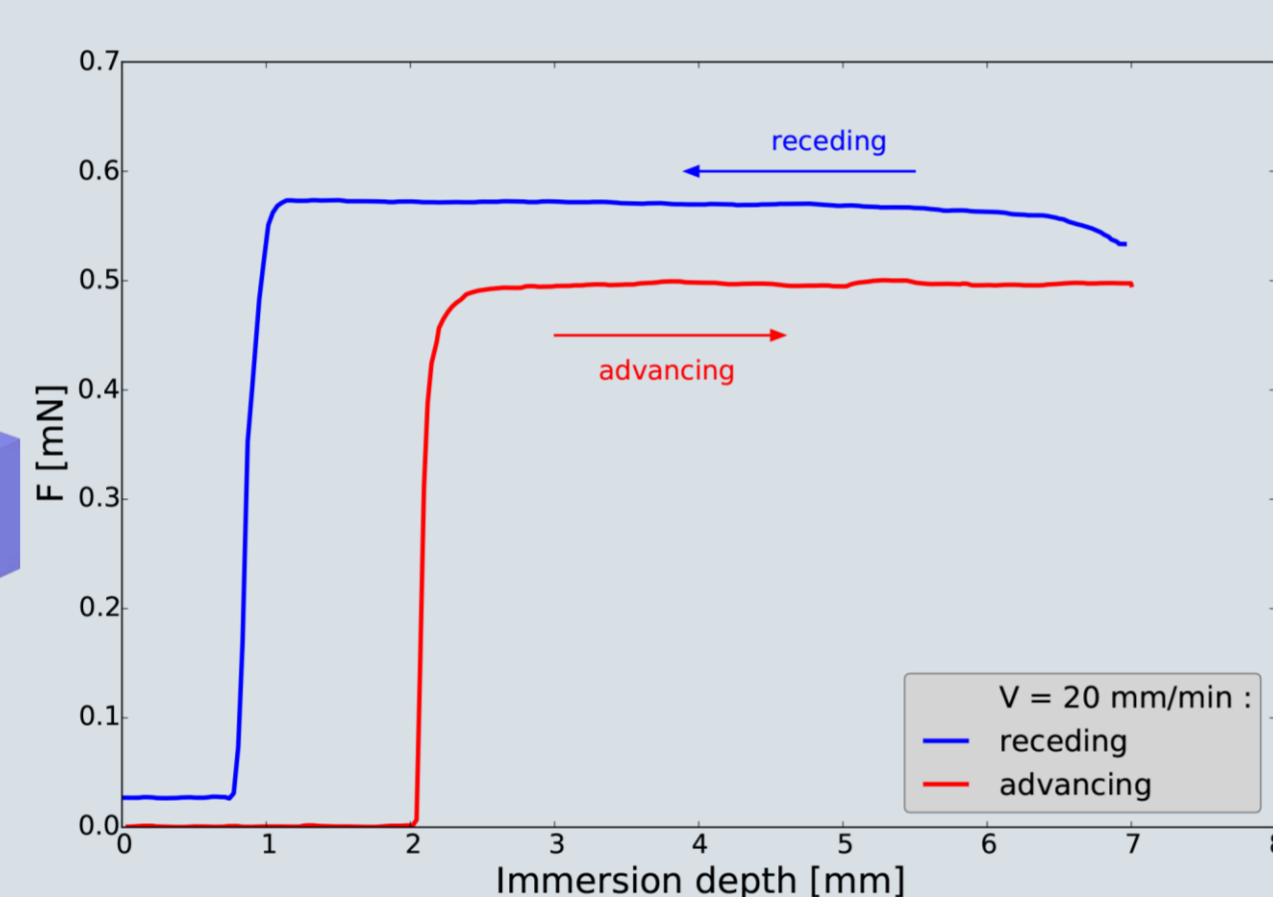
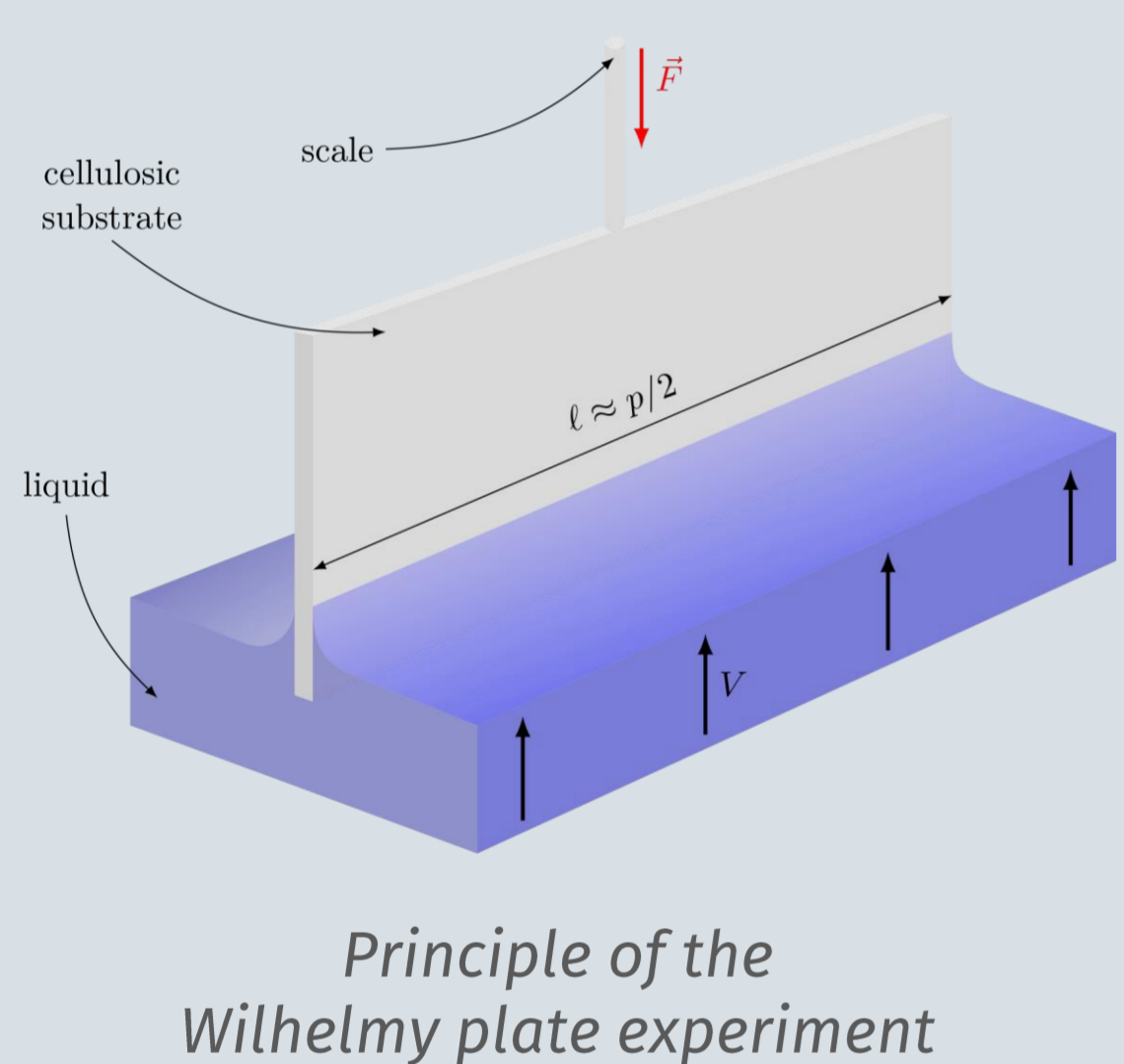
Dynamic wetting models

Characterized by the (dynamic) **contact angle** $\theta \Rightarrow$ unbalanced capillary forces

Model family	Hydrodynamic (HD)	Molecular kinetics (MK)	Combined (MK-HD)
Main parameters	viscosity	intermolecular forces	viscosity + intermolecular forces
Example	Cox-Voinov $\theta^3 - \theta_e^3 = 9\Gamma Ca$	Blake (small angles) $\theta^2 - \theta_e^2 = Ca \left(\frac{v N k_B T}{h K \lambda} \right)$	Petrov $\theta^3 = \theta_c^3(Ca) + 9Ca(\Gamma - C_V)$



Preliminary study



- **Wilhelmy method** (force measurement) on a cellulosic substrate for:
 - Paraffin oils (total wetting)
 - PEG 1450, 3350 and 10000 (partial wetting)
 - Different temperatures (25, 50, 75 °C)
 - Forced wetting: multiple bath velocities ($10^{-4} < Ca < 10^{-1}$, advancing)
- **Materials characterization**
 - Surface tension γ , viscosity η , density ρ (liquids)
 - Roughness, composition (substrates)

A microbalance measures the resulting force F , thus the contact angle:

$$F = \gamma p (\cos \theta - \cos \theta_e)$$

Velocities are expressed with the non dimensional **capillary number** $Ca = \frac{\eta V}{\gamma}$ and plotted against θ for each temperature.

High Ca data is fitted with the **Cox-Voinov** law, giving an estimate for Γ .

We find a **master curve**. The slope change ($1/2$ to $1/3$) around a critical value $Ca = 5 \times 10^{-3}$ shows a transition between MK and HD regimes.

Numerical study

The Wilhelmy plate is reproduced in a **2D FEM** simulation using COMSOL Multiphysics:

- Mesh and parameters are validated (comparison with analytical results)
 - Washburn's law in capillary tubes
 - Spreading of a droplet
- Geometry is wide enough (7 to 8 capillary lengths)
- Materials properties are known (experimental work)
- **Level set** function ϕ (diffuse interface) separating the fluids
- Inlet velocity (Ca) and temperature sweep

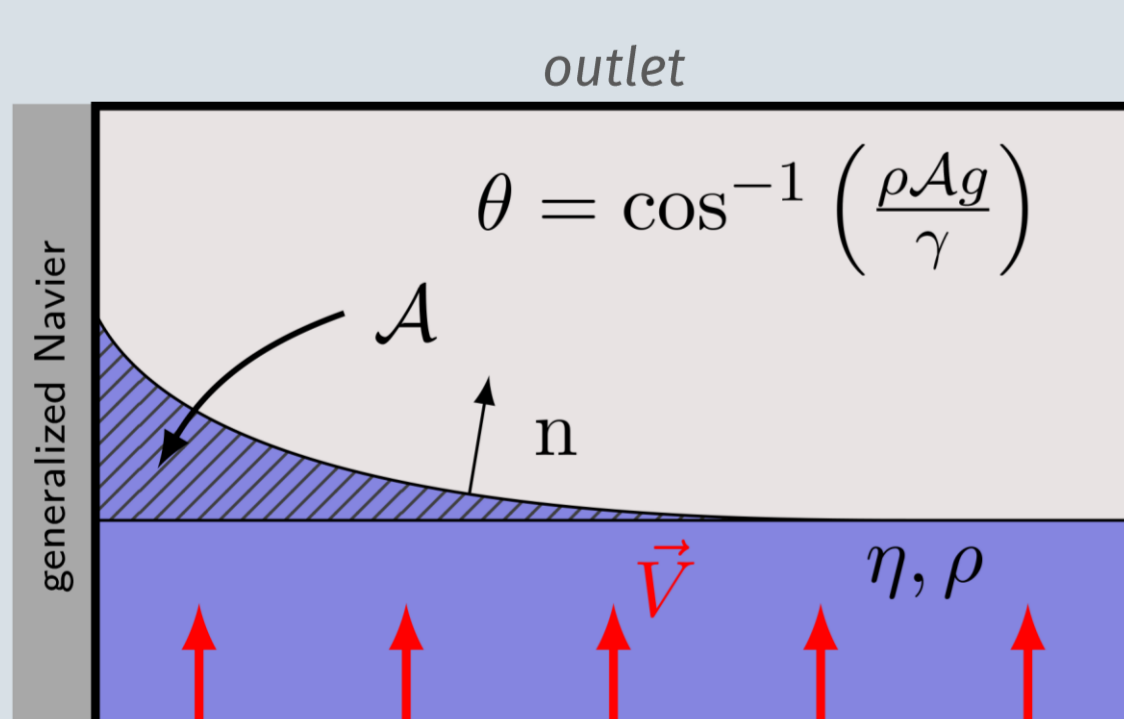
Boundary conditions:

- Symmetry (right), velocity (bottom), no normal stress (top)
- Contact line: generalized Navier slip (*interface formation model*): $n \cdot P(I - nn) + \frac{1}{2} \nabla \gamma = \beta (v_{||}^L - v_{||}^S)$

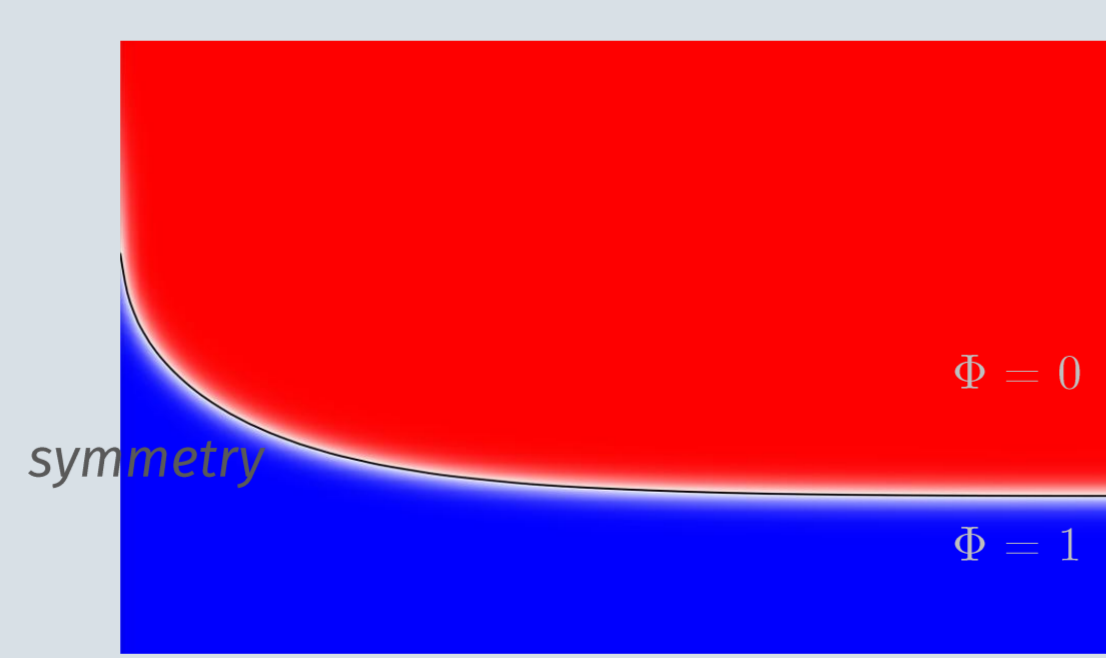
Meniscus area is measured (matching the experimental method) to compute θ .

Above-critical Ca values are fitted with the Cox-Voinov law (HD)

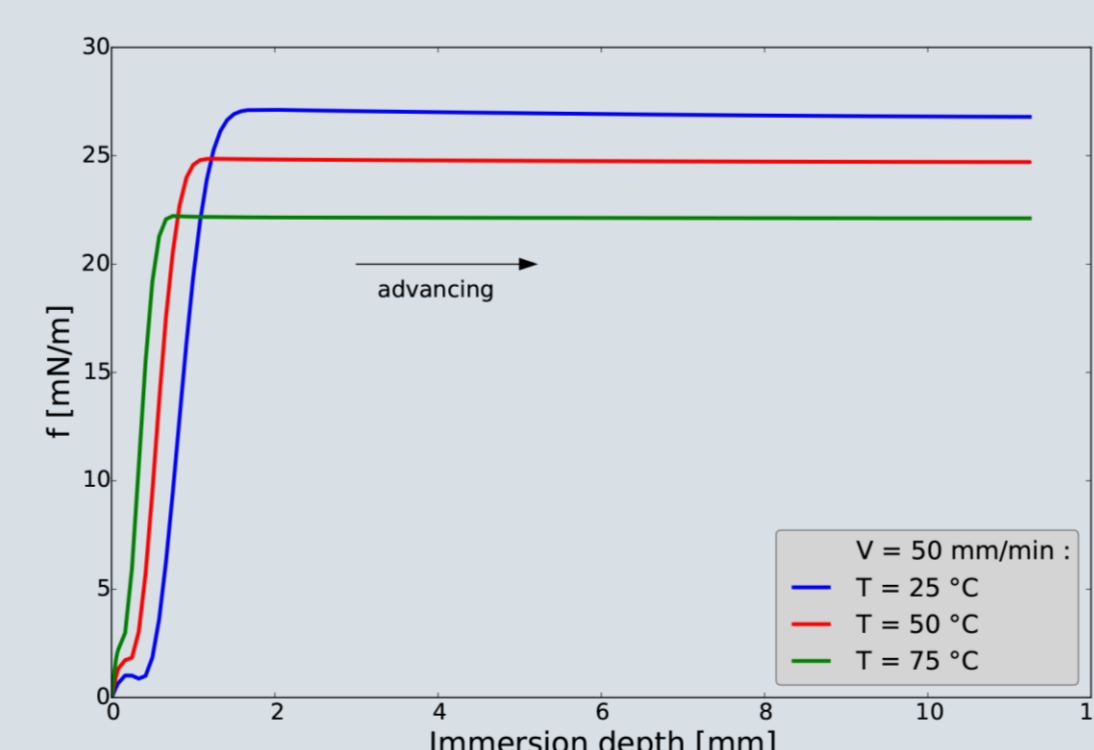
The accuracy of the numerical model is assessed by comparing $\Gamma = \ln \left(\frac{\ell_{max}}{\ell_{min}} \right)$ and its experimental value.



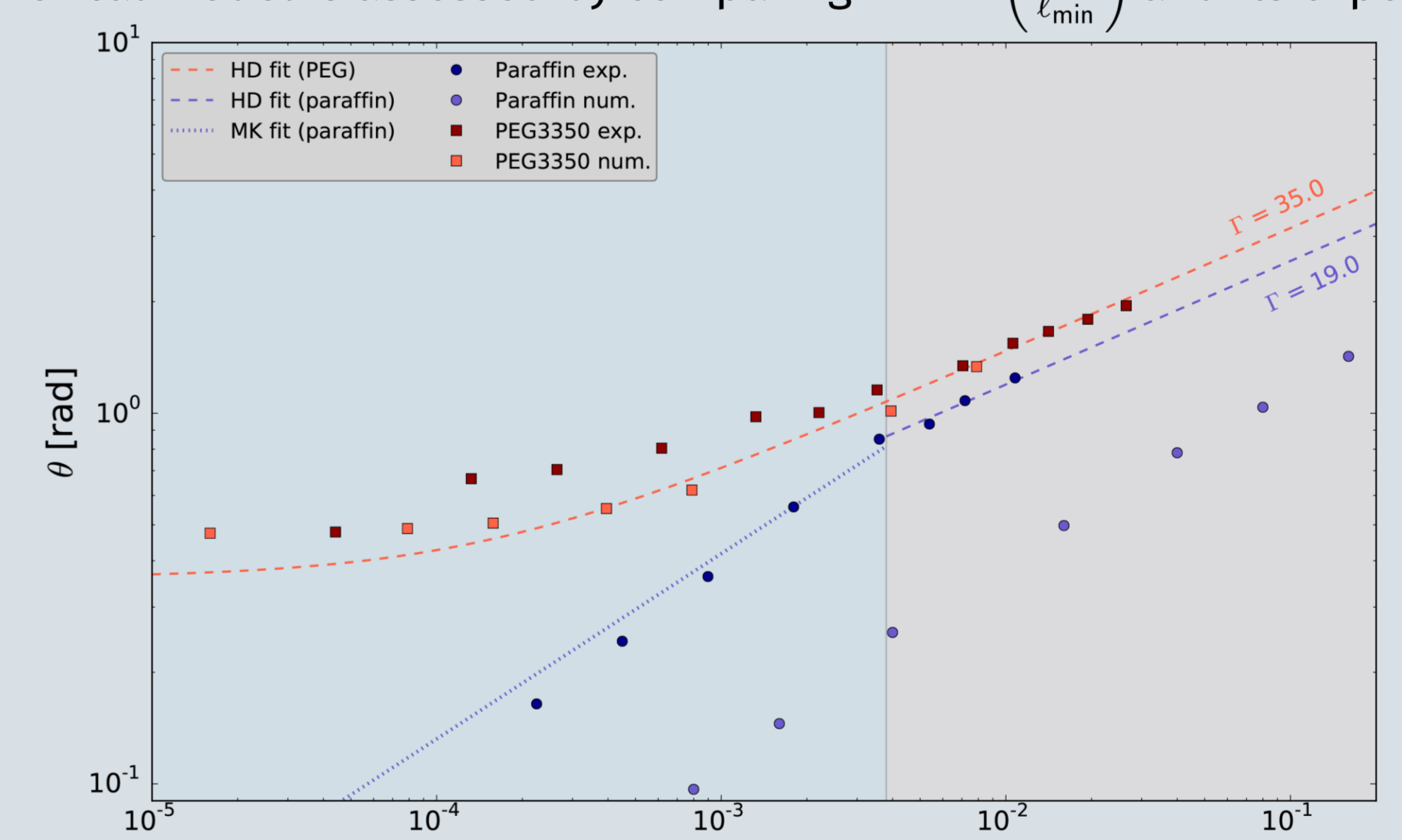
Numerical Wilhelmy plate model setup



Meniscus formed by a paraffin oil for $T=25$ °C and $V=50$ mm/min after 10 s: level set function ϕ



Advancing contact line: evolution of the meniscus weight per unit length



Comparison between experimental and numerical contact angle measurements: 25 °C paraffin oil and 75 °C PEG 3350

The wetting behavior is reproduced. The partially wetting PEG 3350 is in good accordance with the experimental data.

An important shift appears for the totally wetting paraffin oil: while the experimental value of Γ is 19, the numerical model yields a value of 1.9. Further experiments indicate that the model needs a finer mesh for an accurate simulation of totally wetting systems.

Acknowledgements

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Future work

- Finer mesh for total wetting
- Adaptive meshing
- Influence of molar mass
- Cylindric geometry (fibers)
- Larger scale (tow)
- Surface rugosity

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