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► **To cite this version:**

Valentin Rougier, Monica Francesca Pucci, Moussa Gomina, Joel Breard. Dynamic wetting of cellulosic substrates by model liquids. 14èmes Journées d'Etude des Milieux Poreux, Oct 2018, Nantes, France. pp.1, 2018. hal-02395058

HAL Id: hal-02395058

<https://hal.science/hal-02395058>

Submitted on 5 Dec 2019

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Dynamic wetting of cellulosic substrates by model liquids

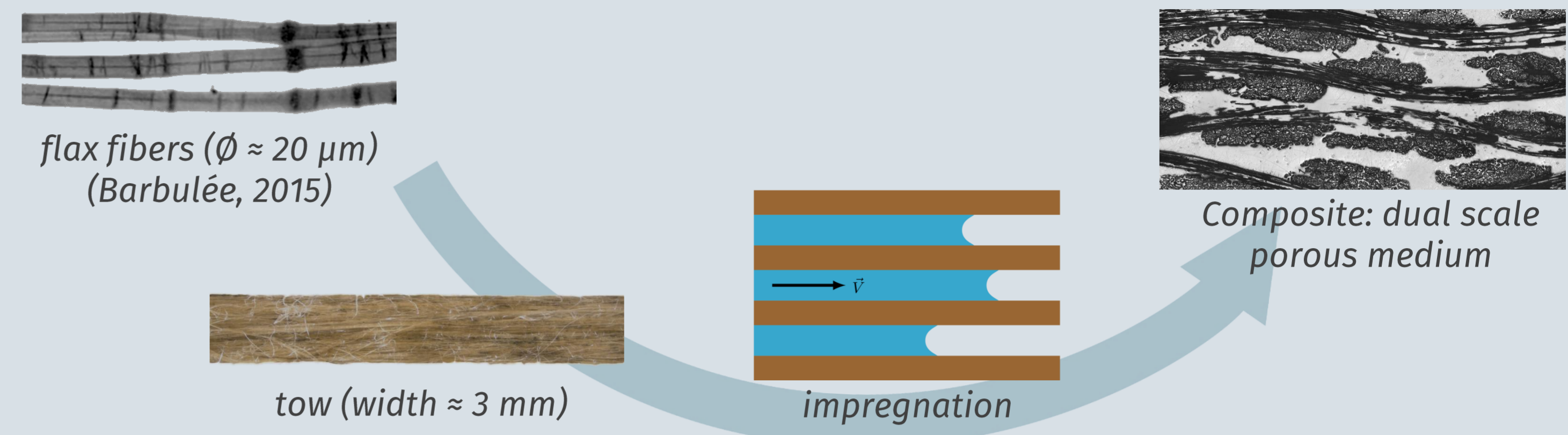
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Motivation

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:

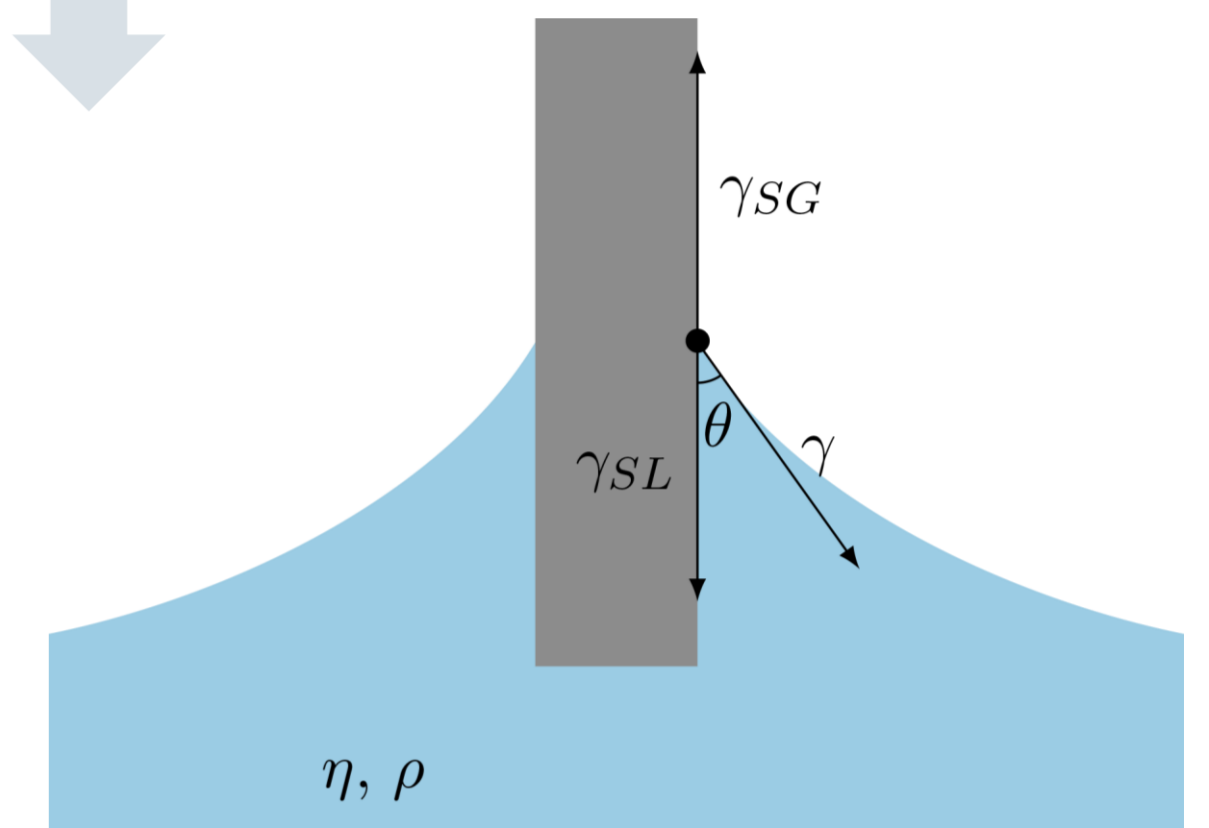
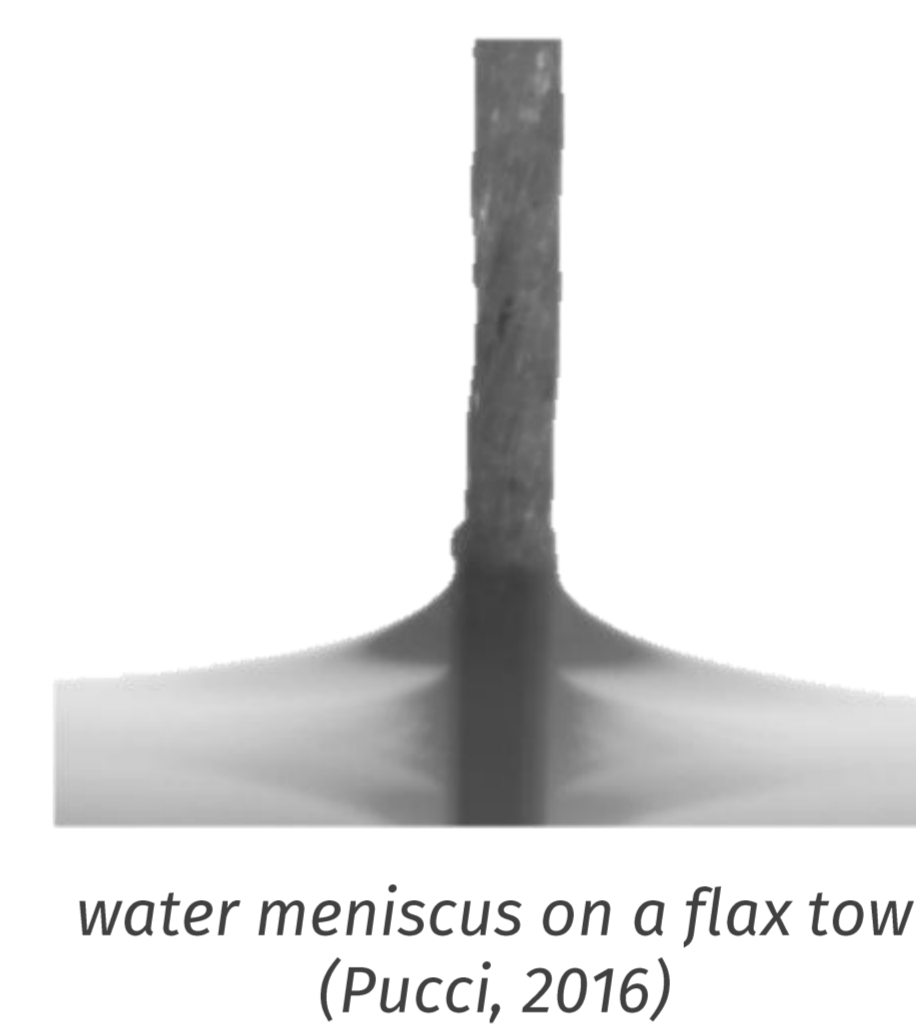
- modeling dynamic wetting phenomena for cellulose-polymer systems
- assessing the influence of physical parameters on dynamic wetting regimes
- evaluating the accuracy of existing models



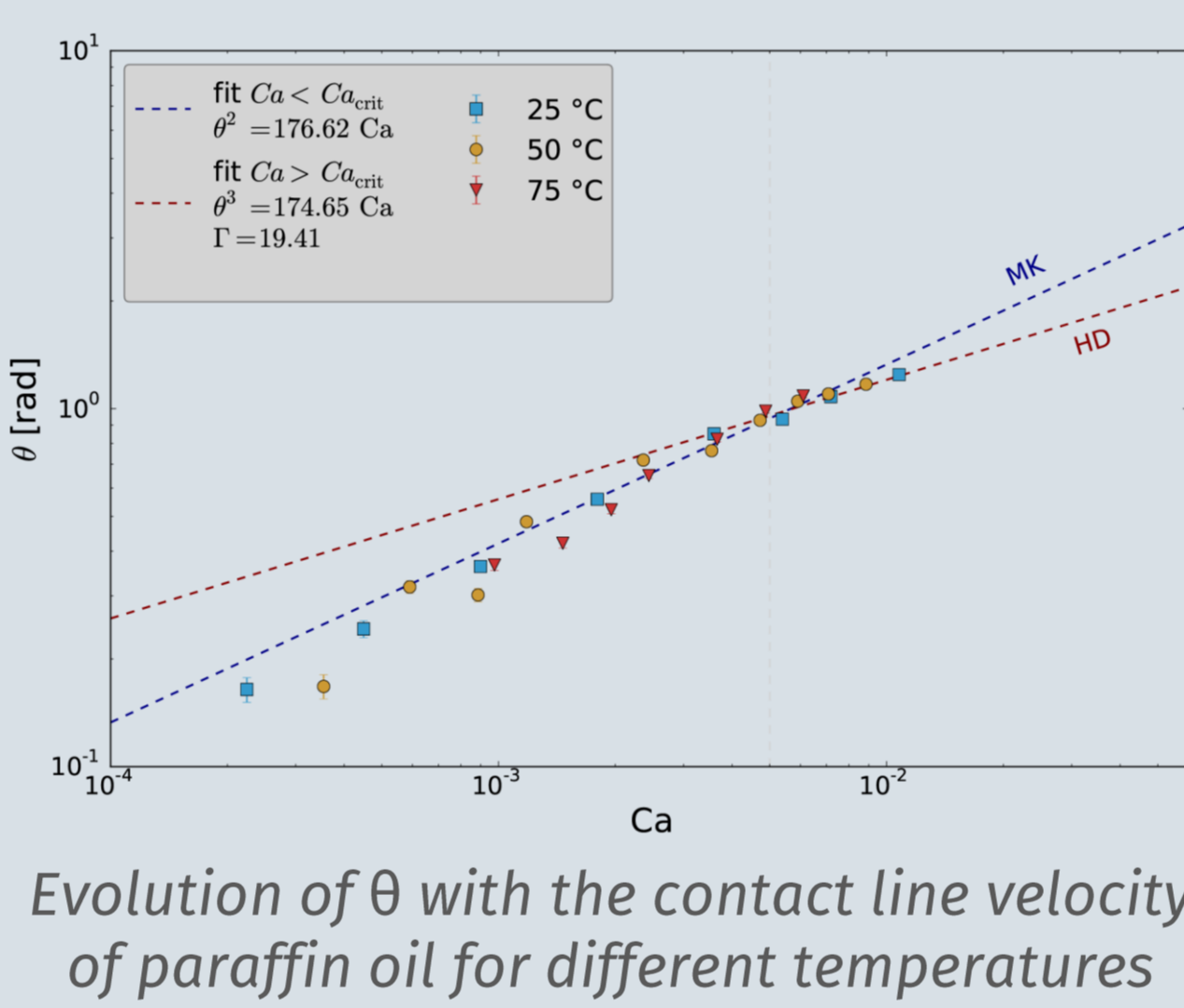
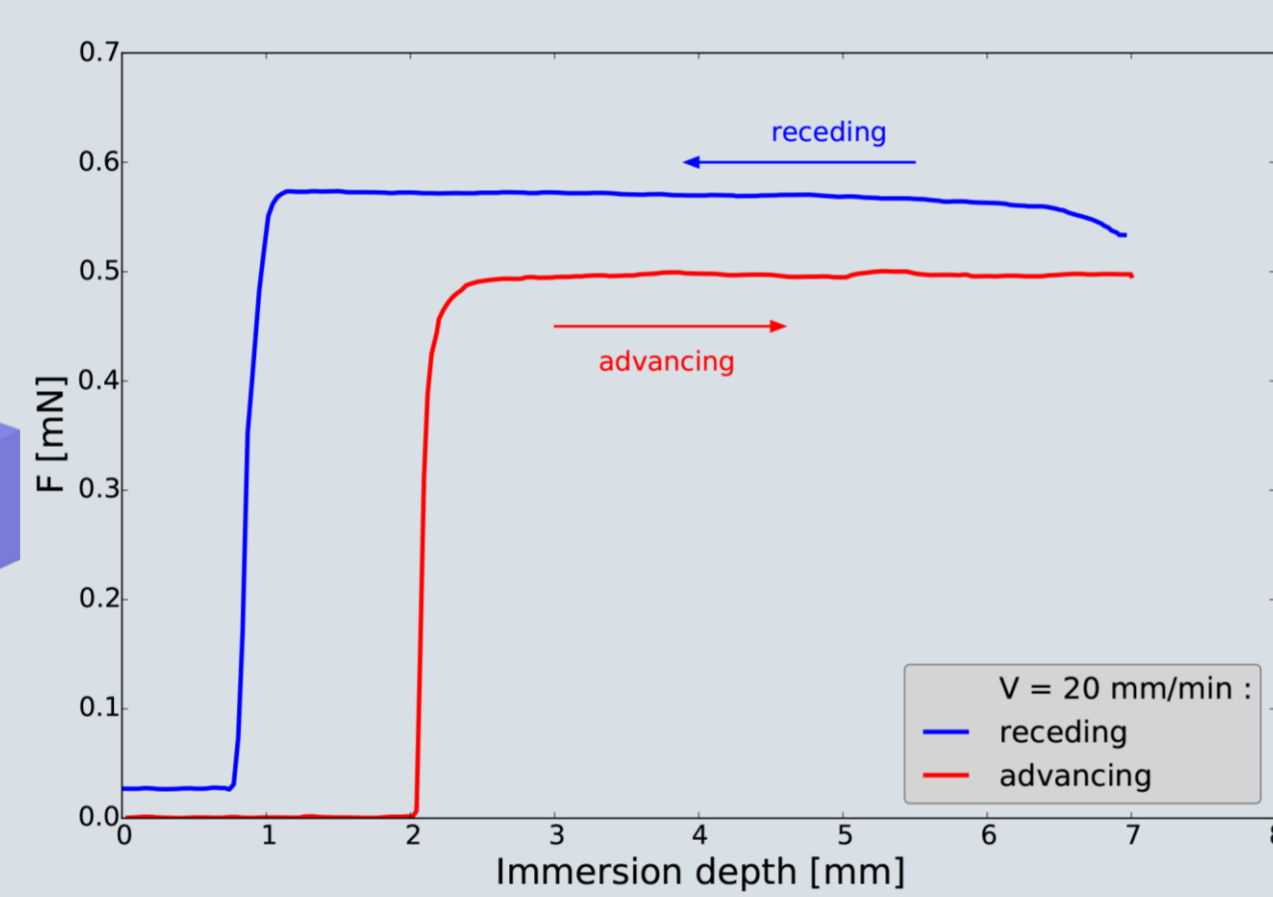
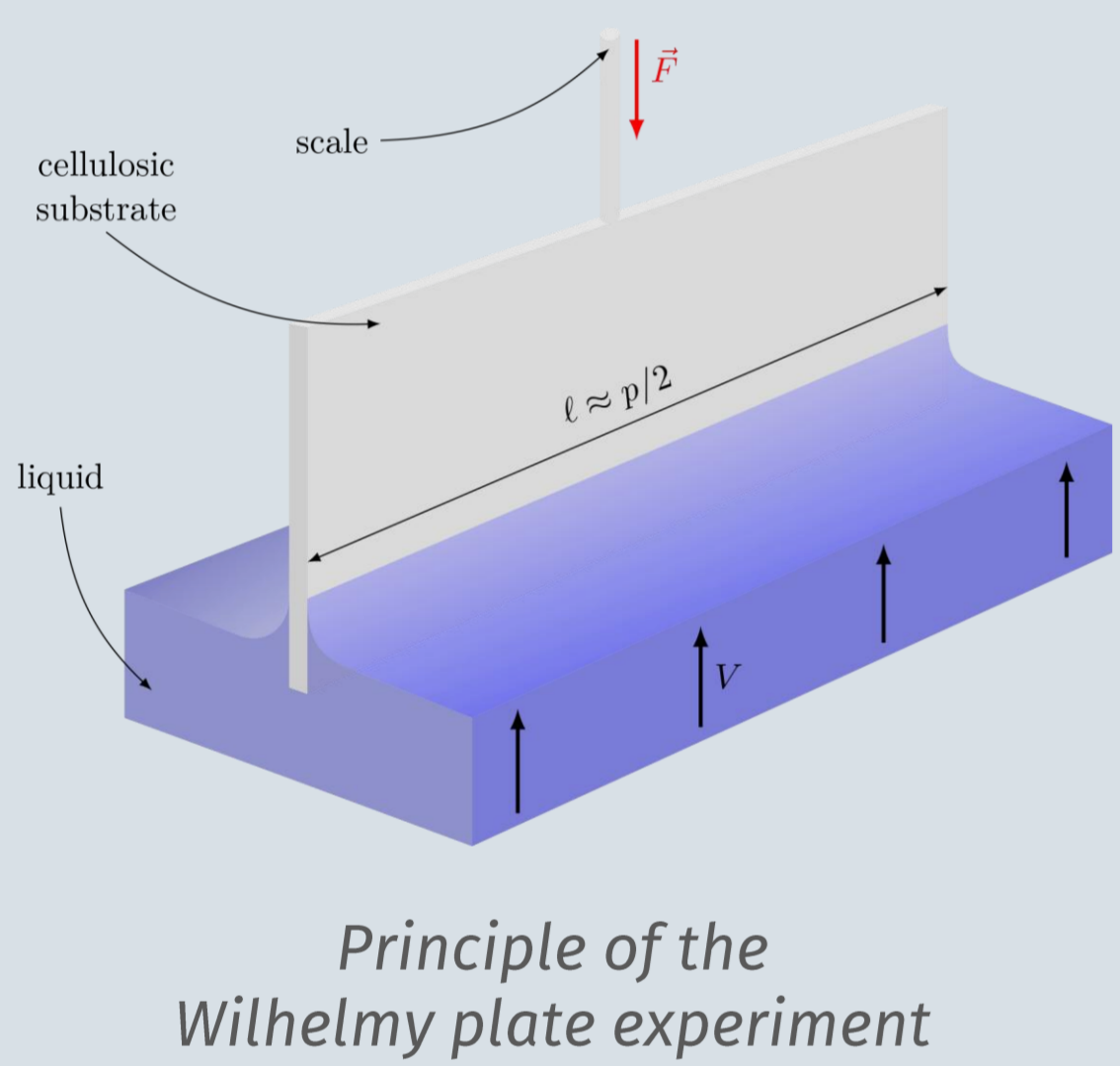
Dynamic wetting models

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

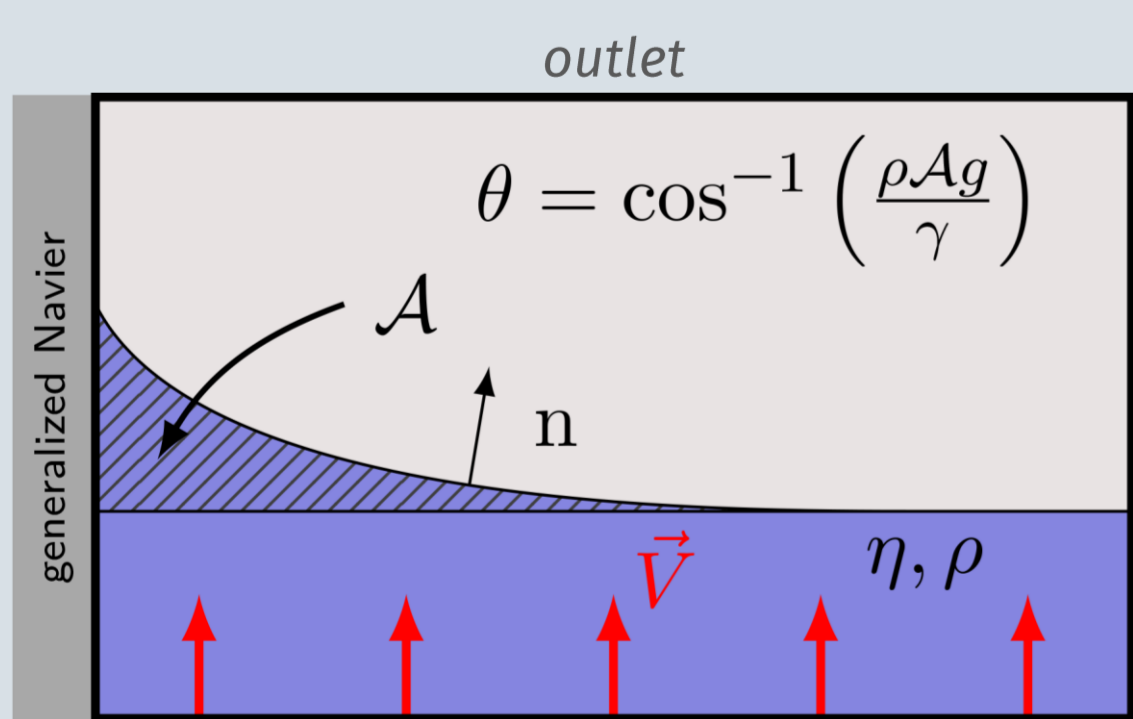
Boundary conditions:

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

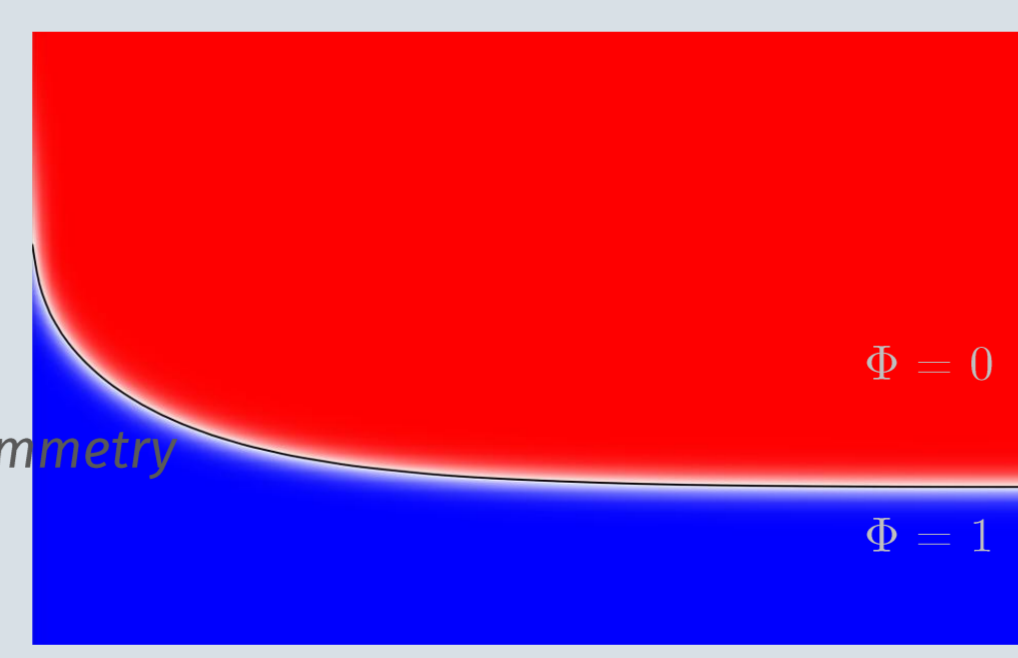
Meniscus area is measured (matching the experimental method) to compute θ .

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

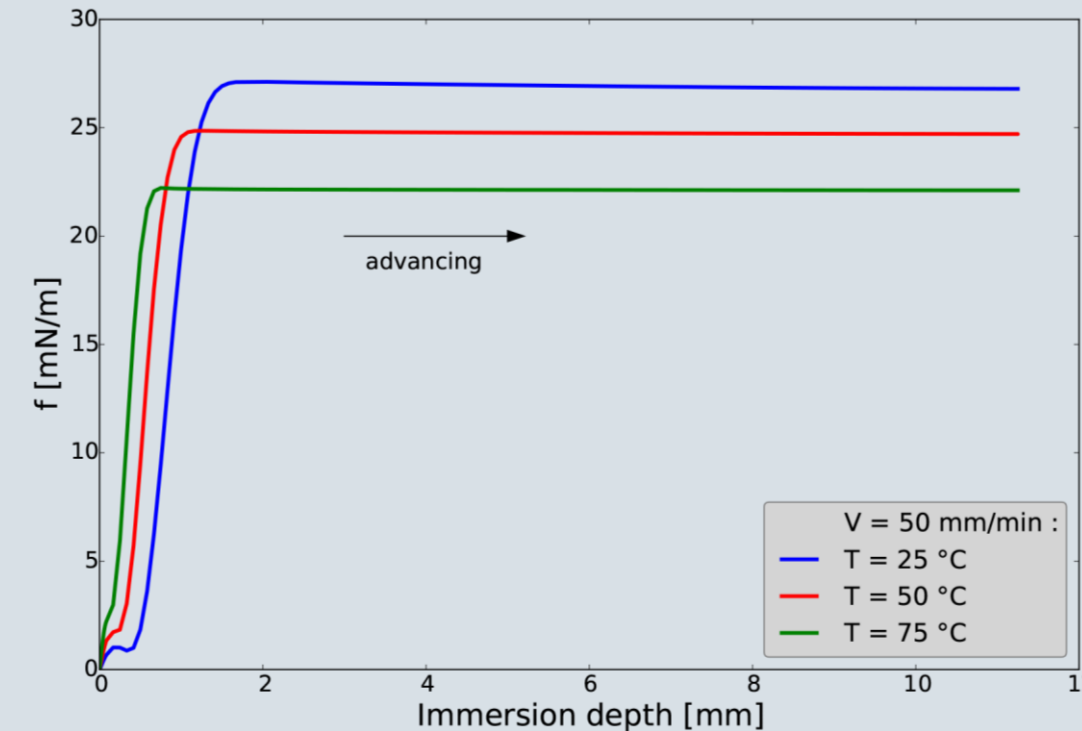
The accuracy of the numerical model is assessed by comparing $\Gamma = \ln \left(\frac{\ell_{max}}{\ell_{min}} \right)$ and its experimental value.



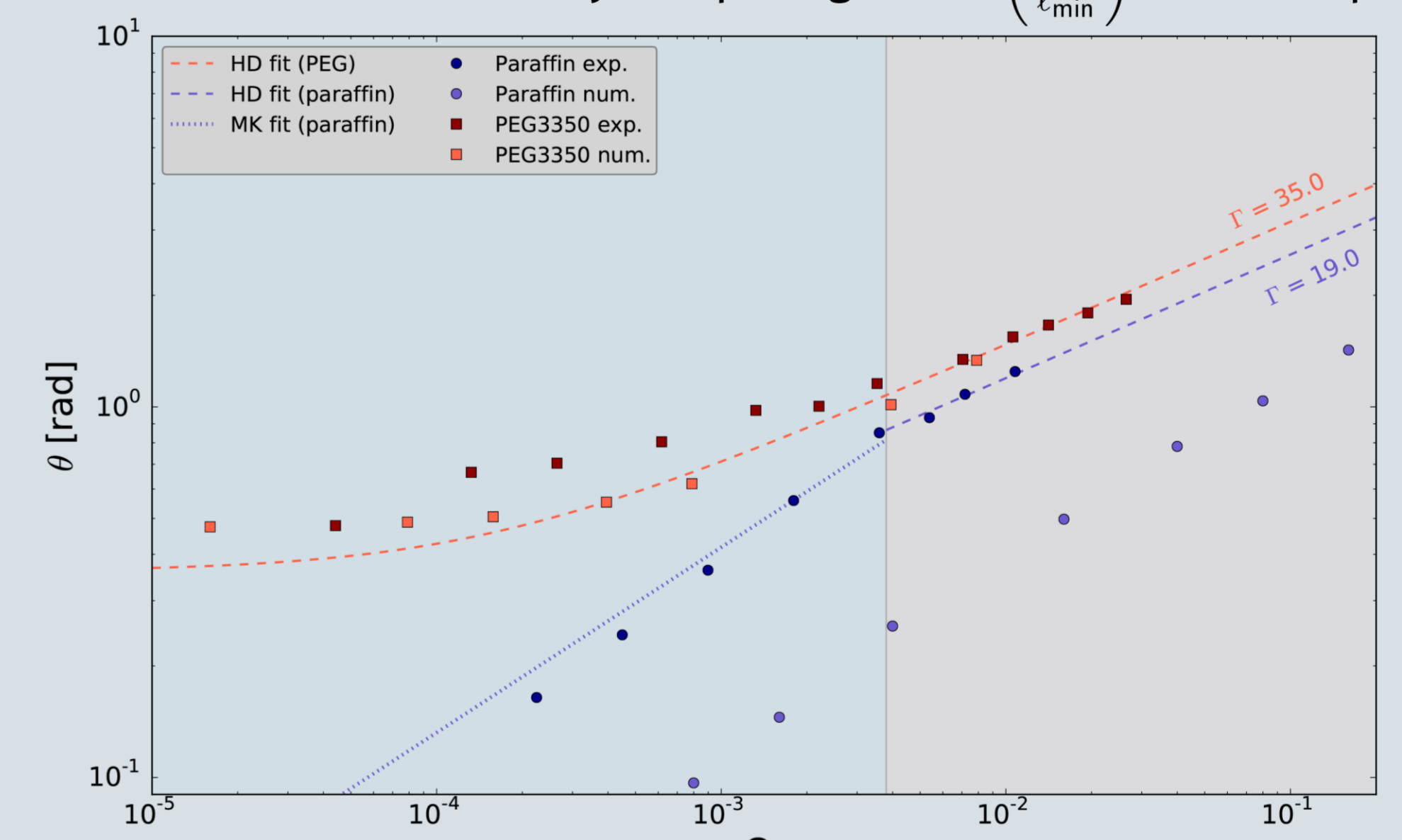
Numerical Wilhelmy plate model setup



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

The authors wish to thank DEPESTELE and bpiFrance for their technical and financial support within the TRAMPLIN program.

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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