Modelling liquid flow structure on a flat surface

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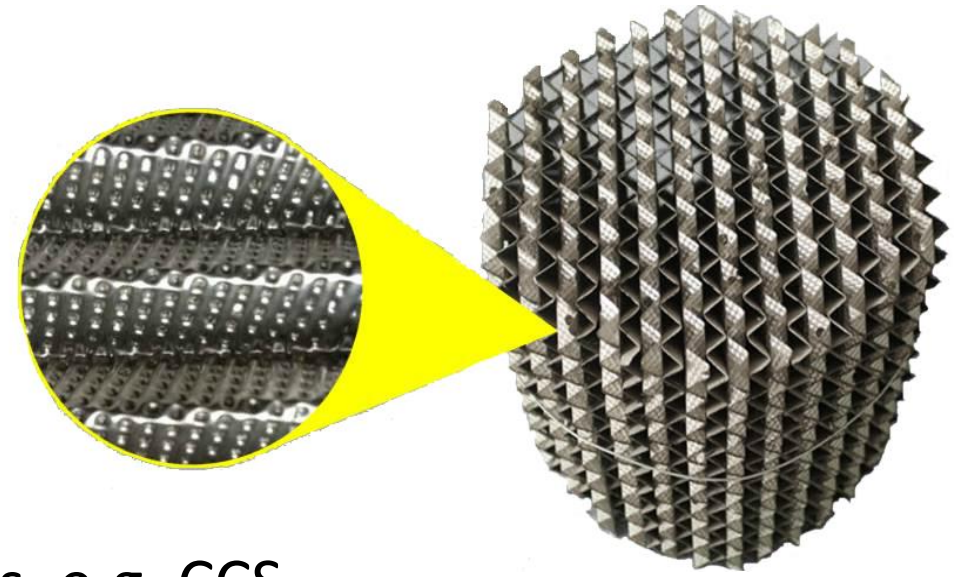
Outline

- Motivation
- Objectives
- Numerical model
- Simulation Results
- Summary

Motivation



- NCN grant - 2-phase flow modelling in complex geometrical structures (random packed beds)

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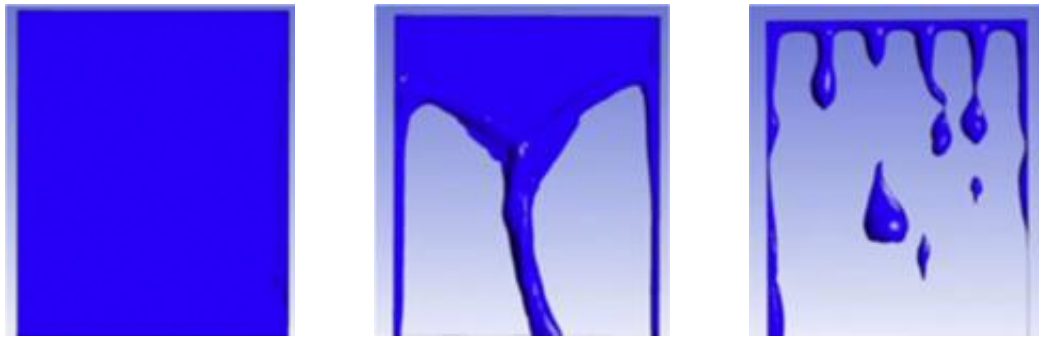
- Packed beds - common in industrial installations, e.g. CCS
- Process (mass, heat, momentum transfer) efficiency strongly dependent on **surface wettability**
- Flow structure:
  - liquid film
  - rivulet flow
  - droplet flow



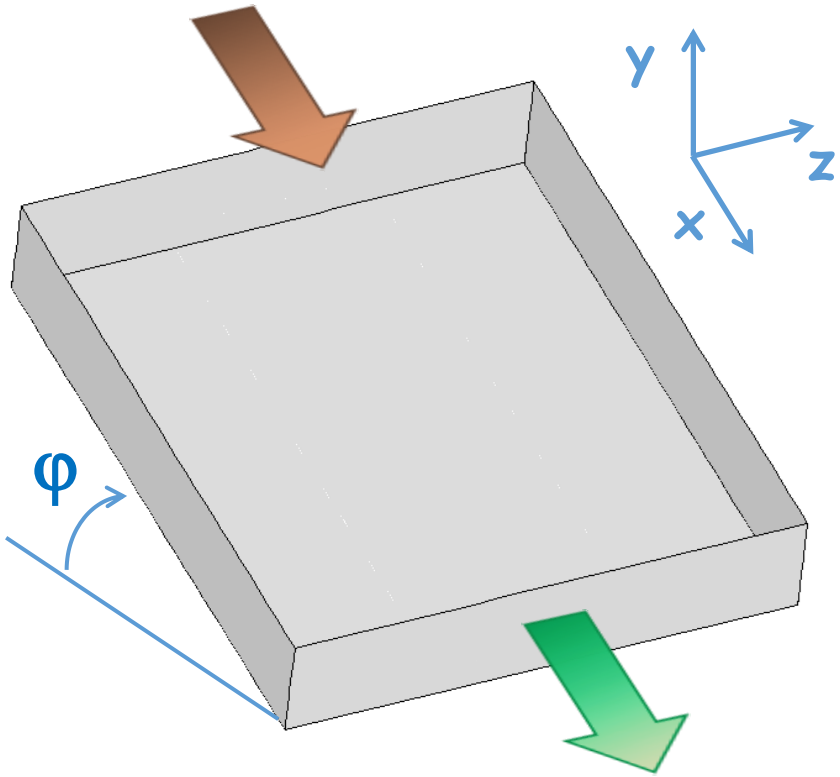
Objectives

- development of a CFD model to simulate the liquid flow structure
- verifying with existing reference data
- researching influence of:
  - contact angle
  - surface tension

Numerical Model

Boundary conditions

velocity inlet BC



pressure outlet BC

dimensions (L/W/H): 60/50/10mm

inclination angle φ = 60

inlet - velocity inlet	**velocity & volume fraction profiles - UDF**
side boundaries - walls	**slip condition, specified shear = 0**
top - wall	
plate - wall	**non-slip condition**
outlet - pressure outlet	**pressure = 0**

Governing equations

2-phase laminar unsteady Eulerian flow model - Volume Of Fluid (VOF)

- continuity equation for the volume fraction

$$\frac{\partial}{\partial t}\left(\alpha_i \rho_i\right)+\nabla\cdot\left(\alpha_i \rho_i U_i\right)=0$$

$$\sum_{i=1}^{n}\alpha_i = 1$$

- material properties

$$\rho = \alpha_L \rho_L + \left(1-\alpha_L\right)\rho_G \qquad \nu = \alpha_L \nu_L + \left(1-\alpha_L\right)\nu_G$$

- momentum equation

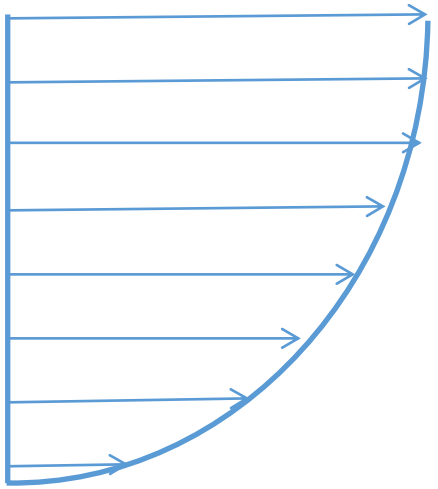
$$\frac{\partial}{\partial t}\left(\rho U\right)+\nabla\cdot\left(\rho UU\right)=-\nabla p+\nabla\cdot\left[\mu\left(\nabla U+\nabla U^T\right)\right]+\rho\vec{g}+F$$

Governing equations

$$F = \sigma \frac{\rho \cdot \kappa \cdot \nabla \alpha_L}{0.5\left(\rho_L + \rho_G\right)}$$

$$\mathrm{Re} = \frac{\rho_L \cdot U_L \cdot \delta}{\mu_L}$$

water - air	
surface tension	72mN/m
contact angle	70°
plate's material	Steel



- liquid film theory

$$\delta_L = \left(\frac{3\left(\mu_L / \rho_L\right)^2}{g \sin\varphi} \mathrm{Re}_L \right)^{1/3}$$

⇒ parabolic velocity profile ⇒ UDF ⇒ Boundary conditions

UDF – User Defined Function

Computational resources

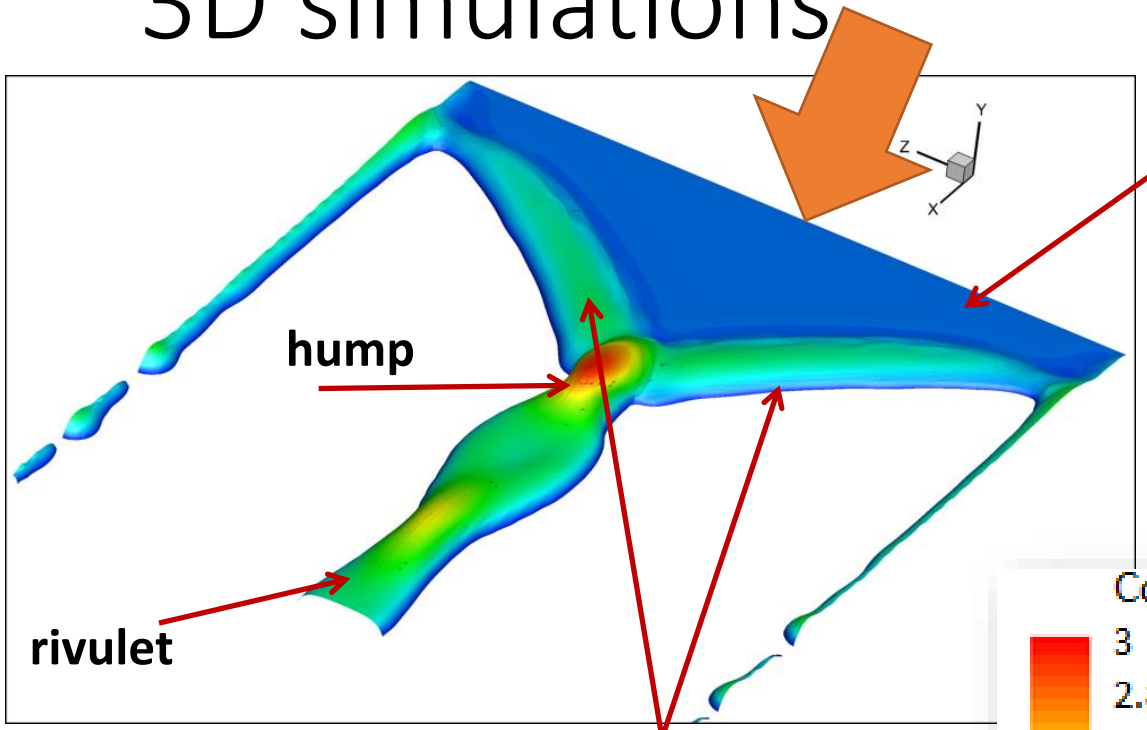
The research was calculated with use of Prometheus cluster available thanks to Cyfronet Pl-Grid Infrastructure.

Mesh size: 4 mln nodes

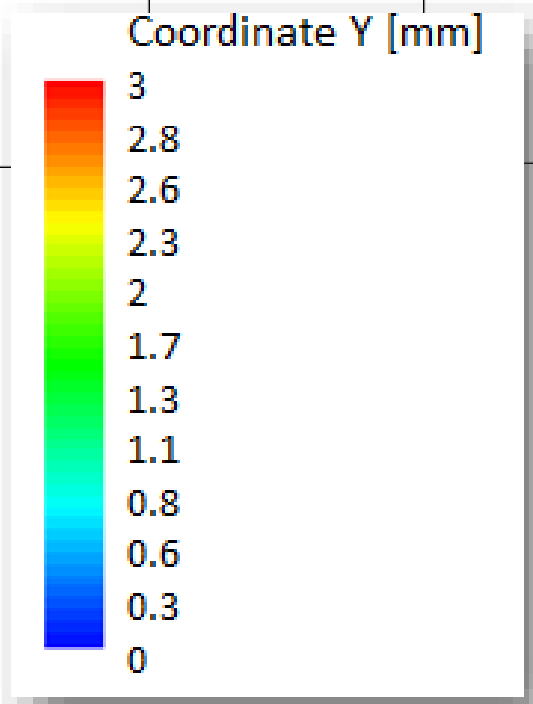
Minimum required numer of time steps: 15000

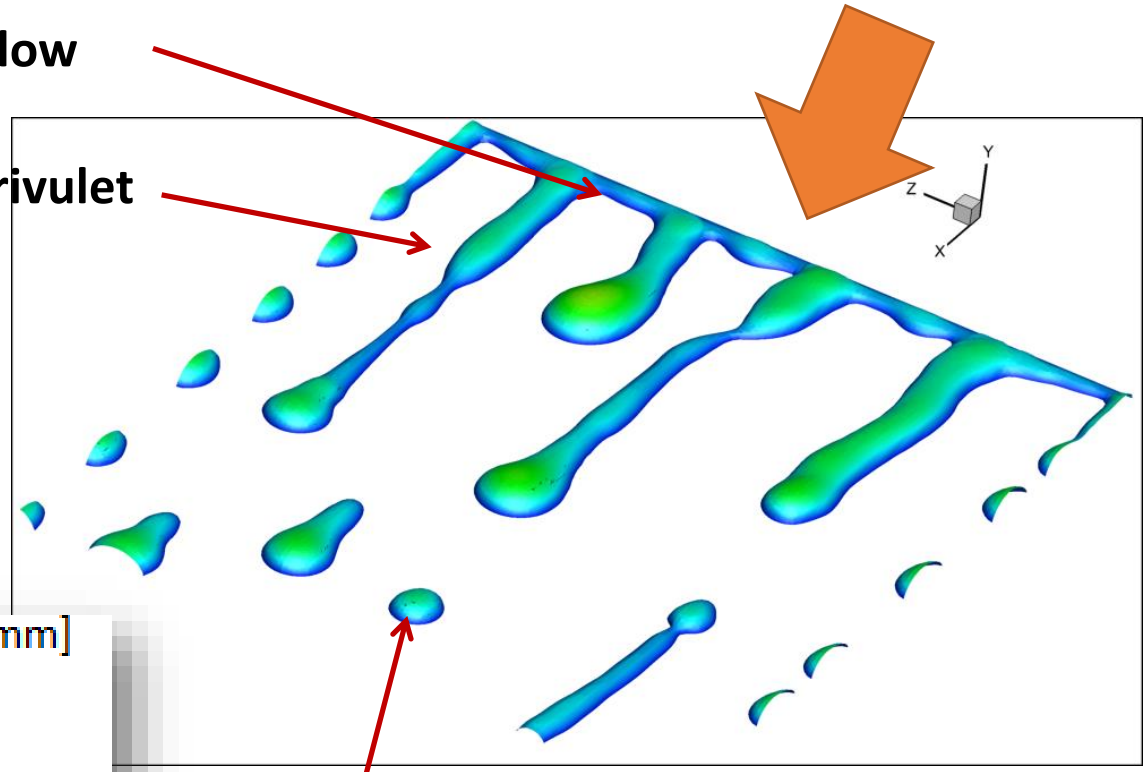
Amount of used processors	Needed time for one time step
1 (standard computer)	45 minutes
6 (cluster)	9-15 seconds

3D simulations



flow structure - Re = 100

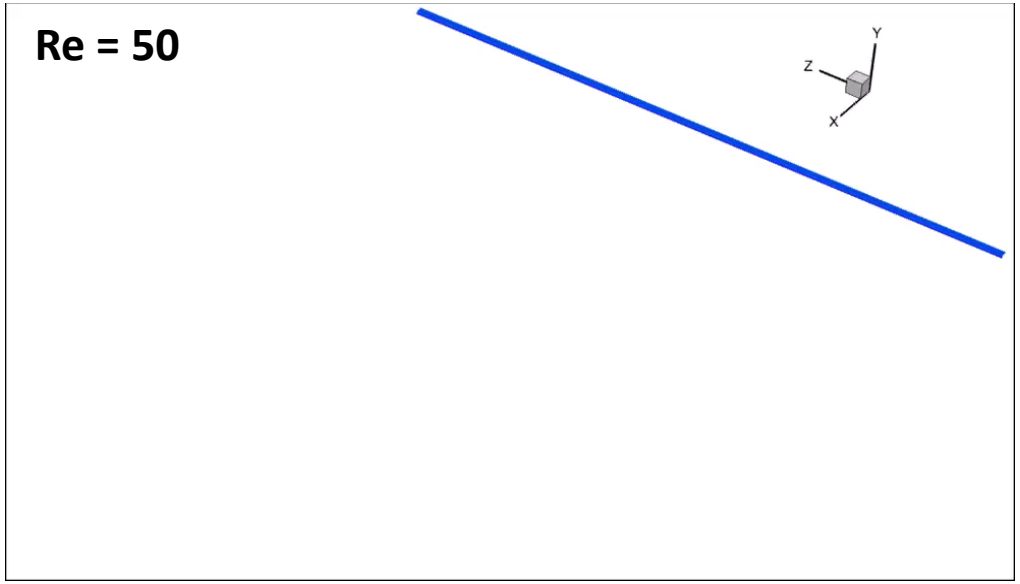




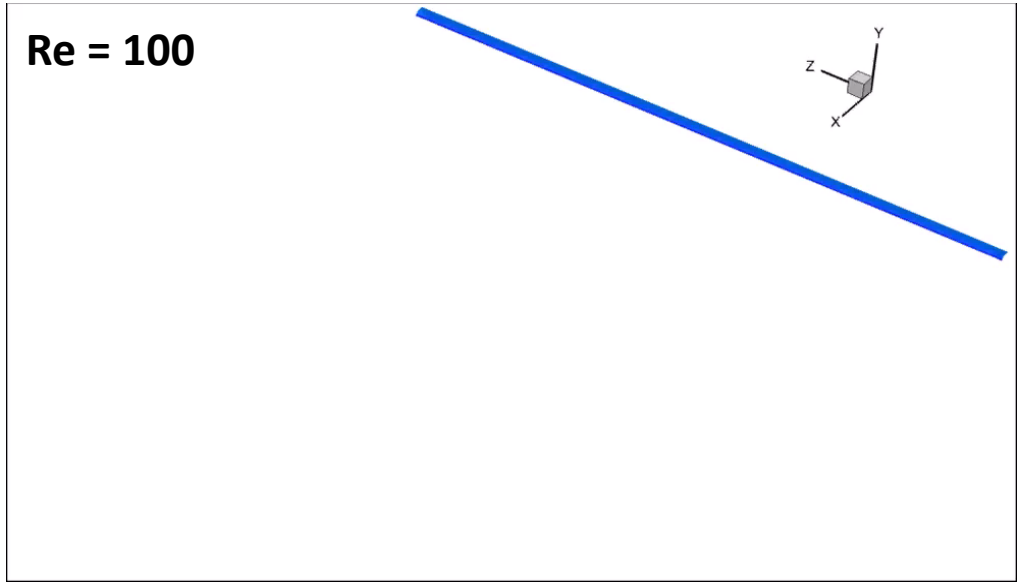
flow structure - Re = 50

Results for different Reynolds numbers

Re = 50

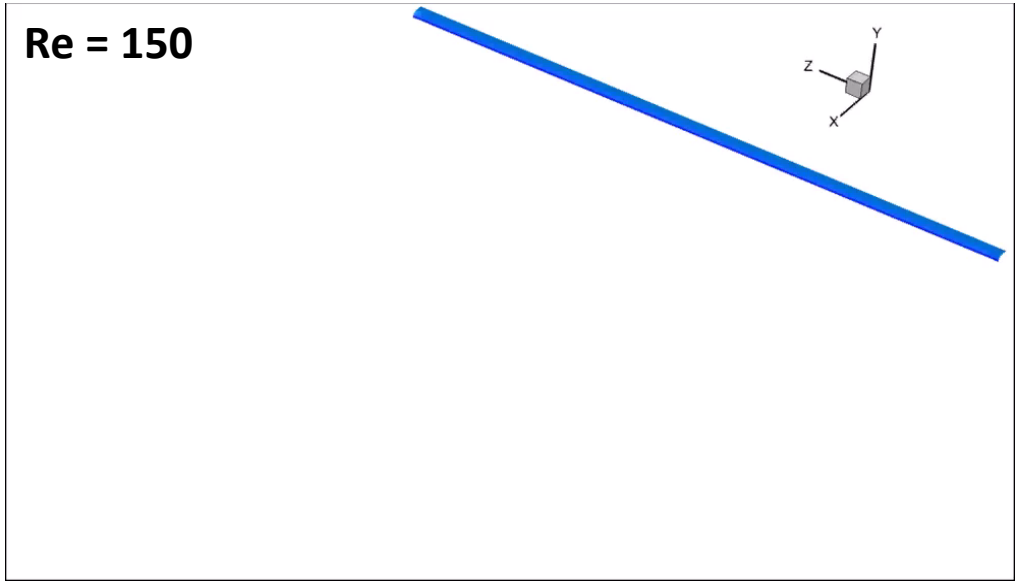


Re = 100



Re = 55

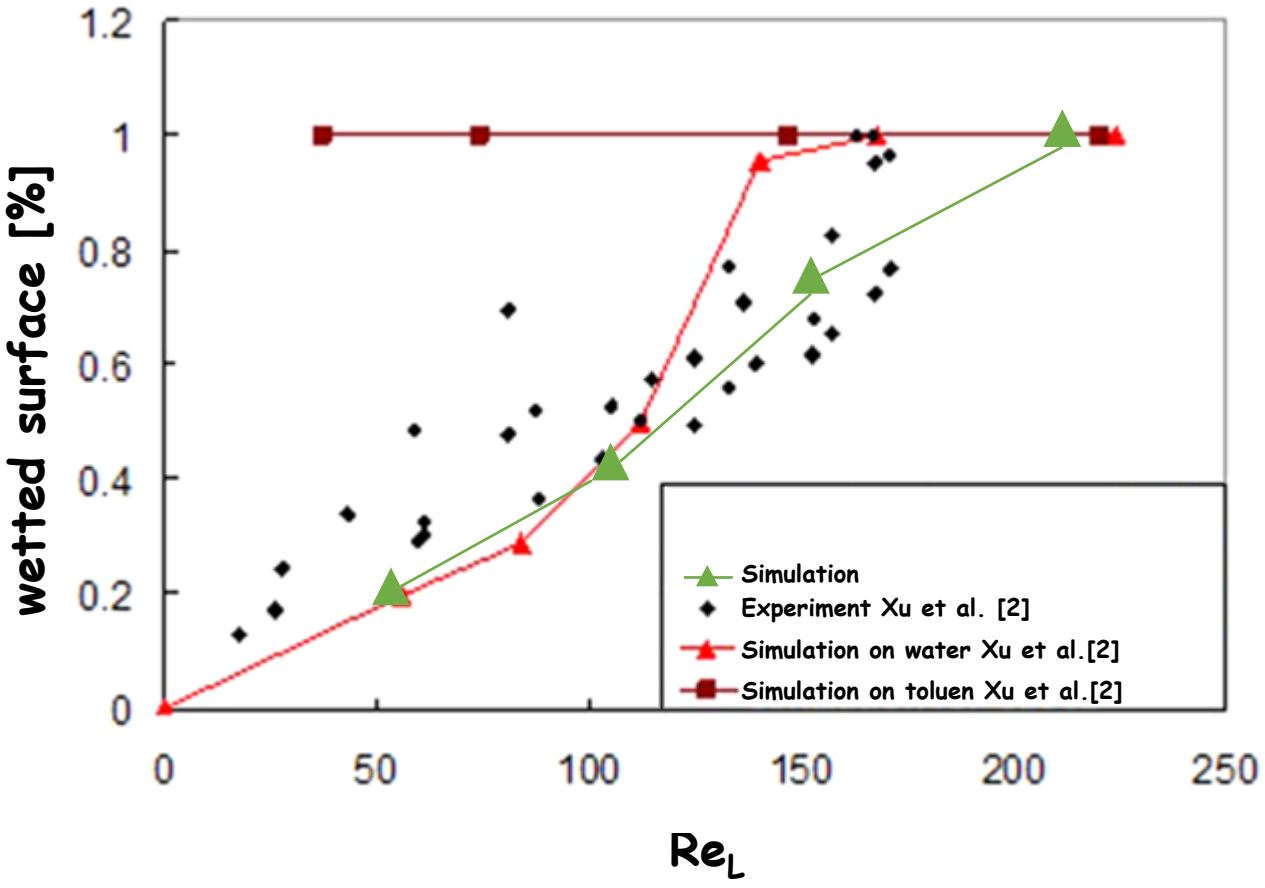
Re = 150



Re = 112,5

1) Haroun Y. et al.Chemical Engineering research and design, 2014, vol. 92, p 2247–2254

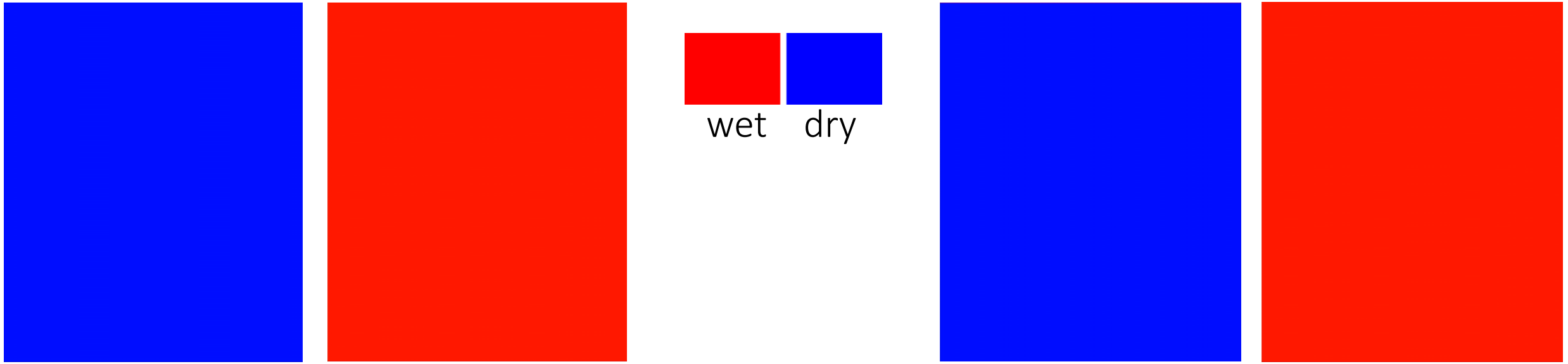
Influence of Reynolds number

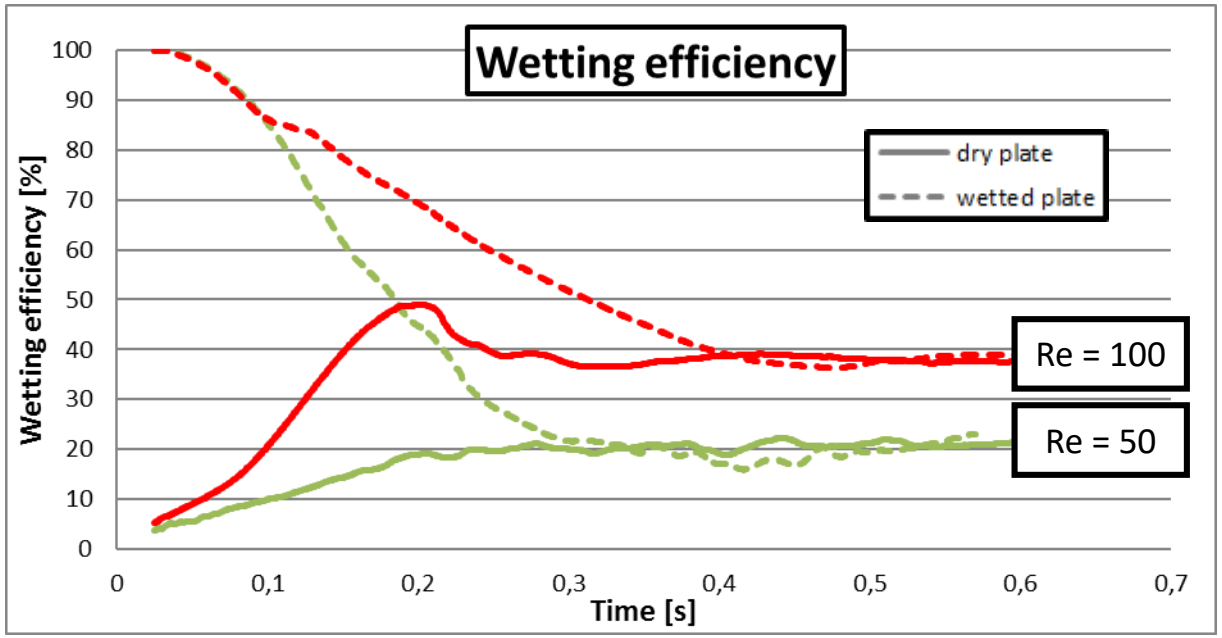


very good consistant with literature data

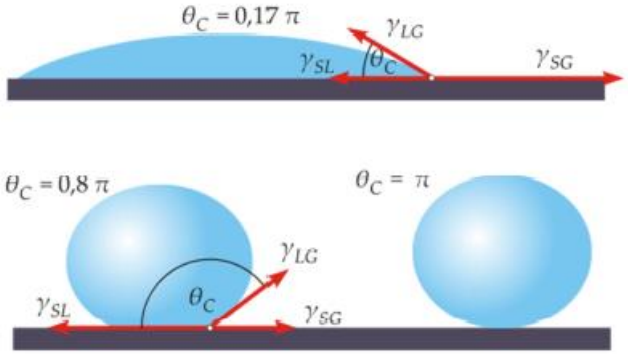
2) Xu Y. Y., Zhao M., Paschke S., Wozny, G.: "Detailed Investigations of the Countercurrent Multiphase (Gas−Liquid and Gas−Liquid−Liquid) Flow Behavior by Three-Dimensional Computational Fluid Dynamics Simulations", Ind. Eng. Chem. Res. 2014, vol. 53, p. 7797−7809

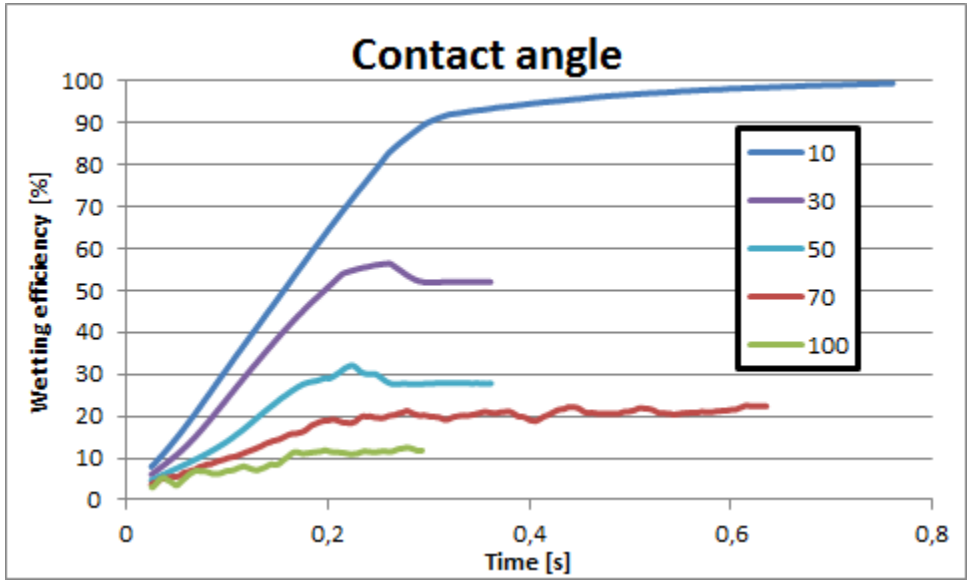
Results for different initialization method



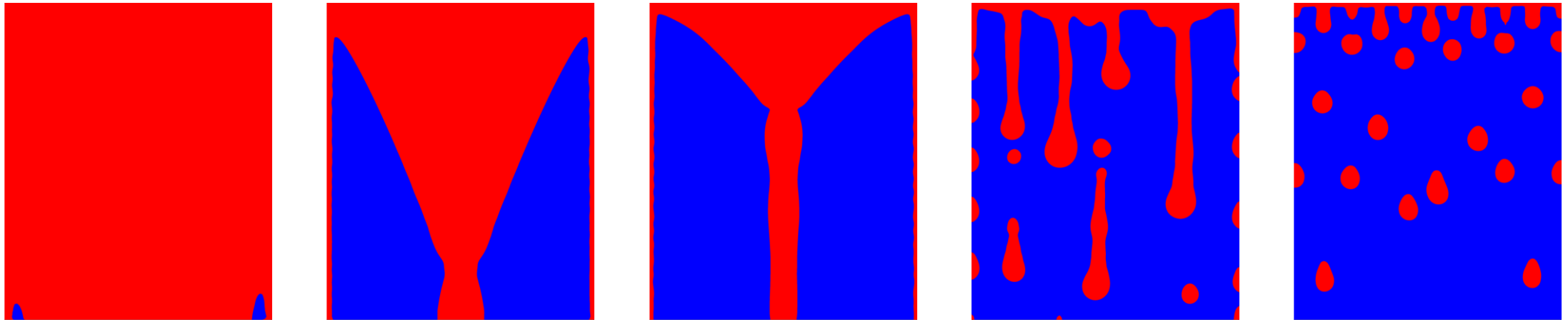


Contact angle impact





Re = 50

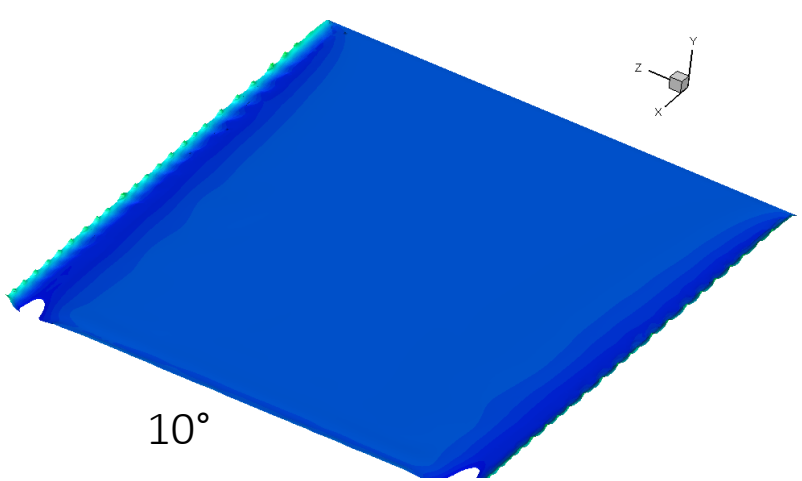


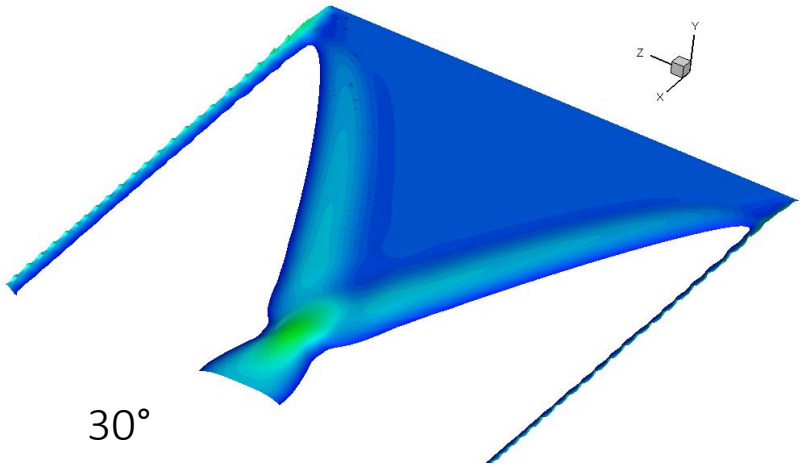
10° 30° 50° 70° 100°

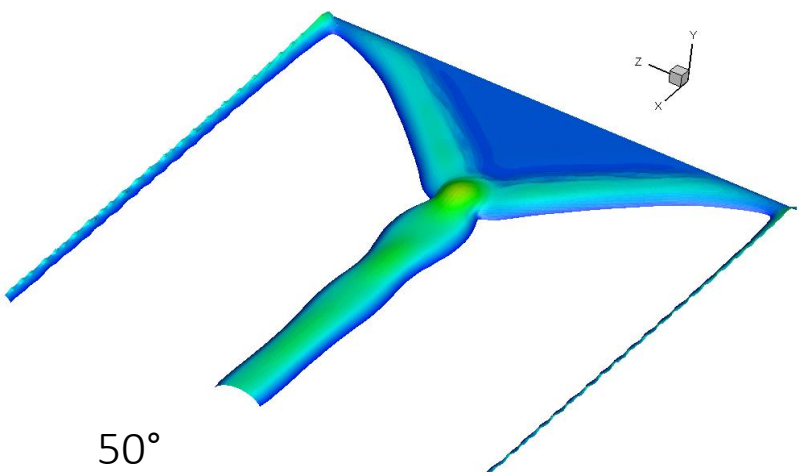
http://www.chemistryexplained.com/elements/L-P/Mercury.html
https://commons.wikimedia.org/wiki/File:Krople.svg

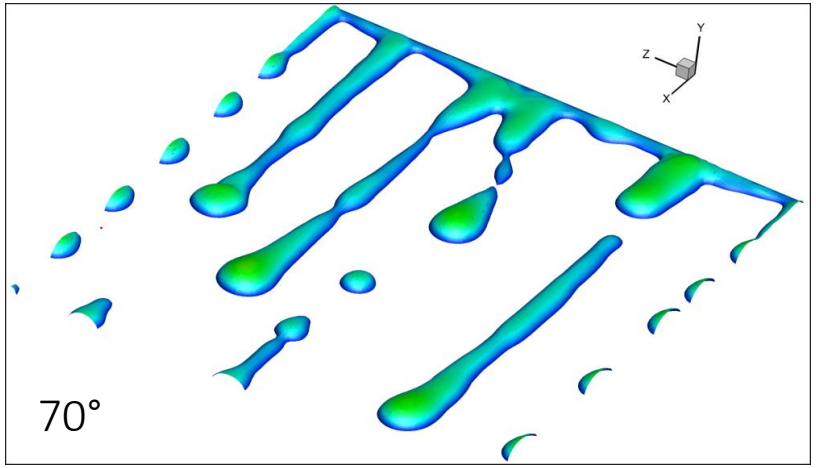
Contact angle impact

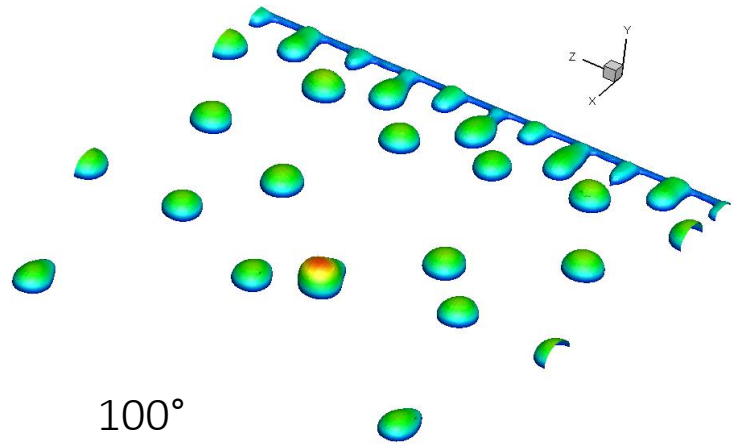
Re = 50



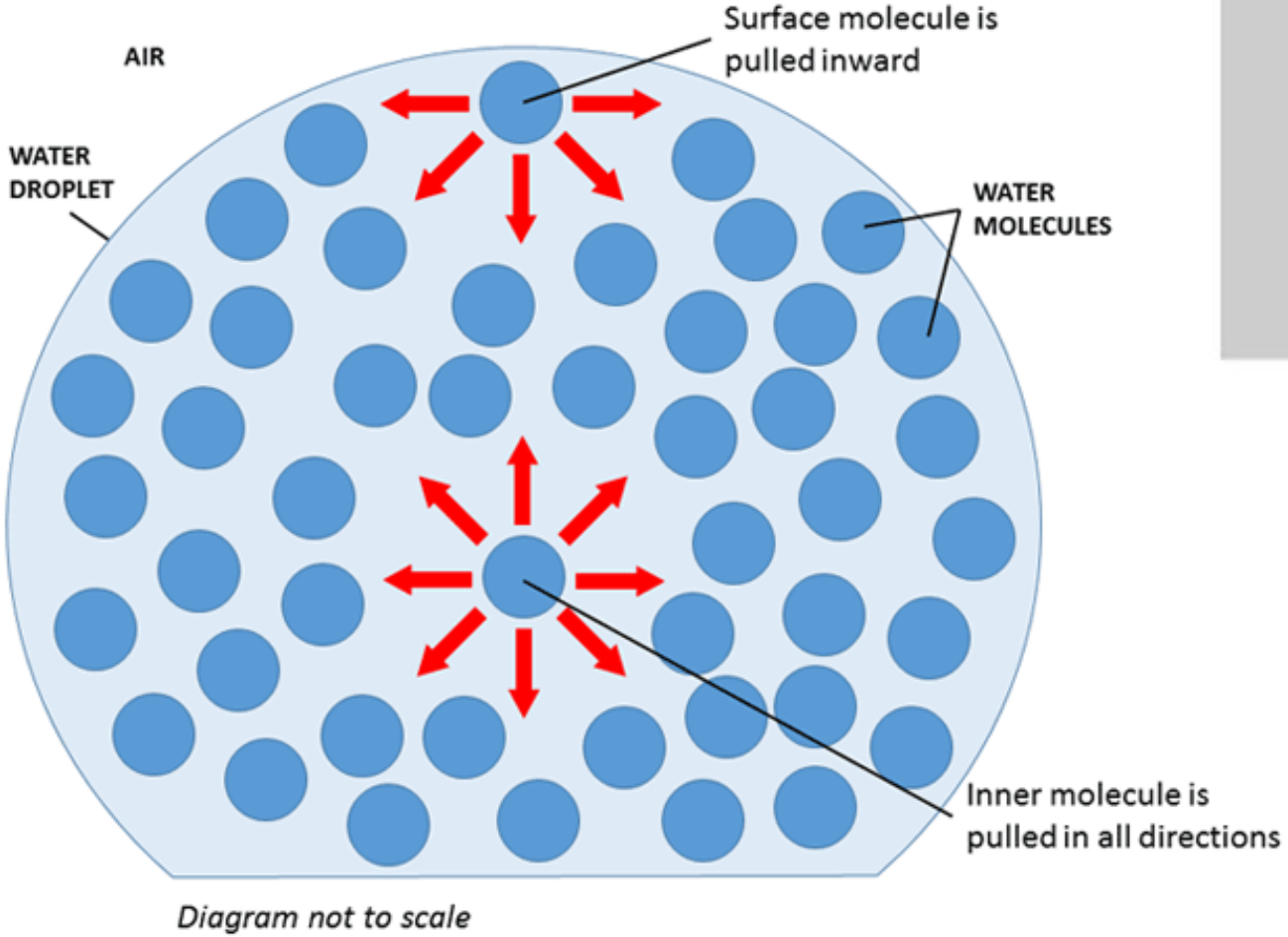


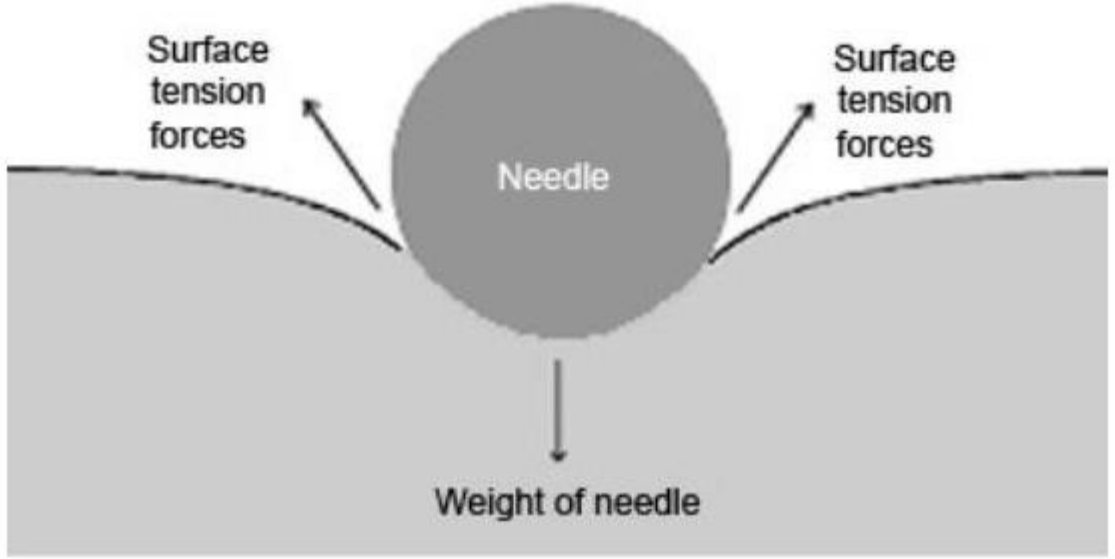






Surface tension impact

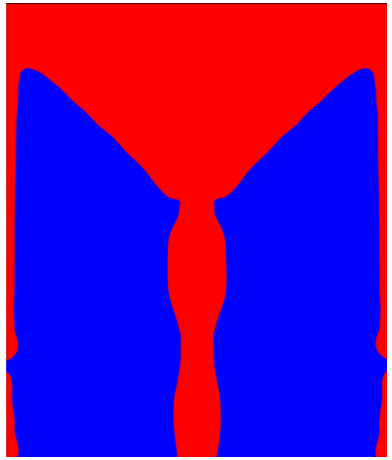




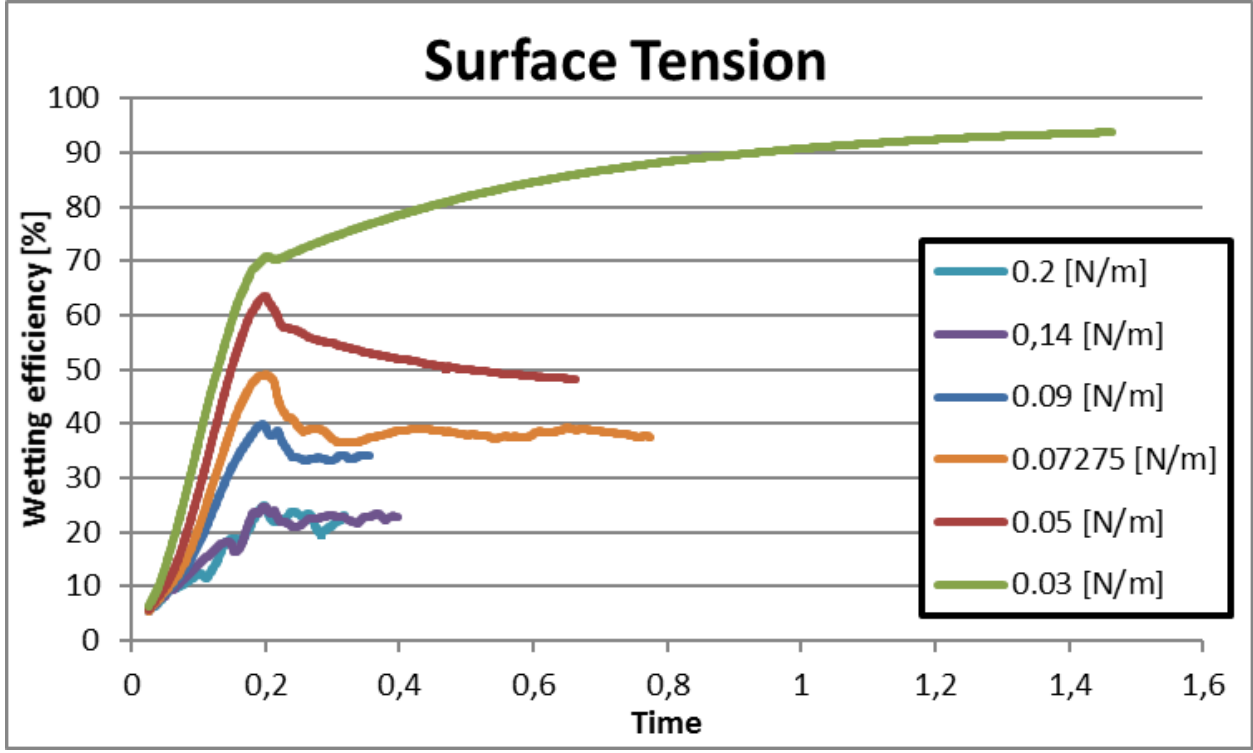
http://www.sciencebuddies.org/science-fair-projects/project_ideas/Chem_p021.shtml#background
http://www.rsc.org/learn-chemistry/resource/res00001719/detergents-soaps-and-surface-tension?cmpid=CMP00005233
https://simple.wikipedia.org/wiki/Surface_tension

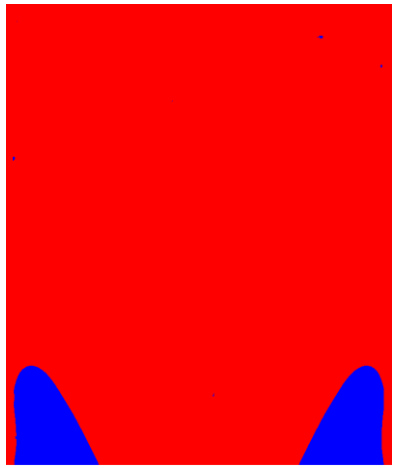
Surface tension impact

Re = 100

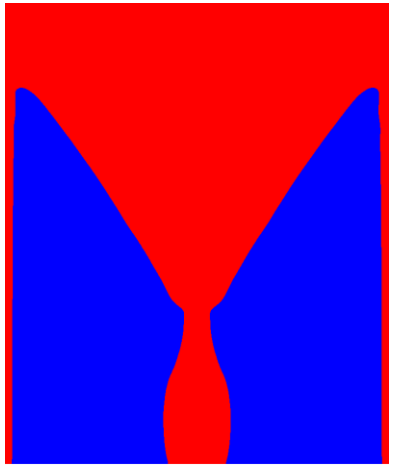


0.07275 $\left[\frac{N}{m}\right]$

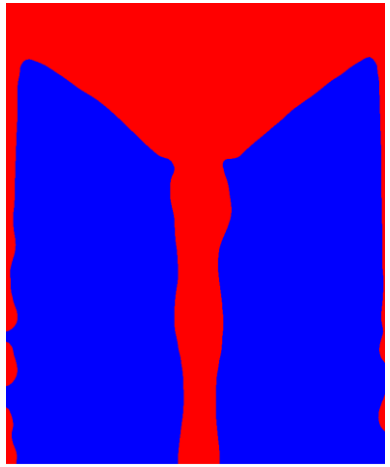




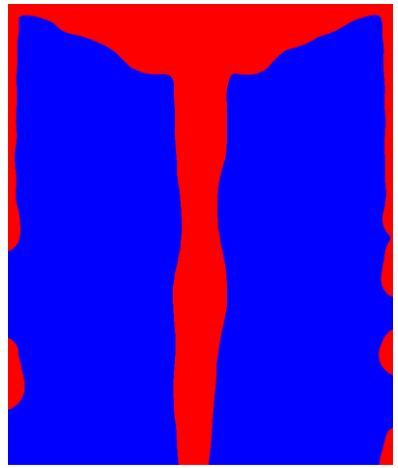
0.03 $\left[\frac{N}{m}\right]$



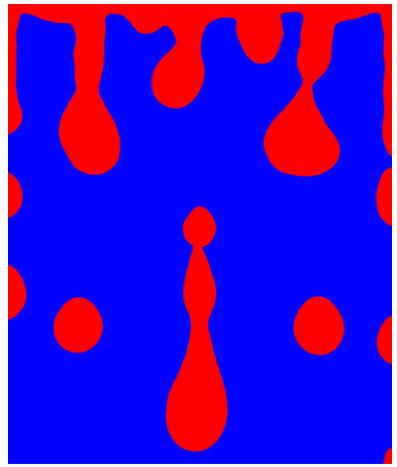
0.05 $\left[\frac{N}{m}\right]$



0.09 $\left[\frac{N}{m}\right]$



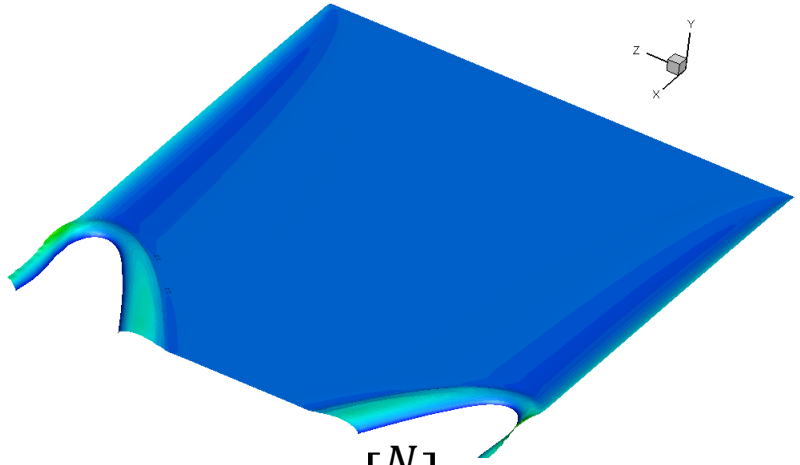
0.14 $\left[\frac{N}{m}\right]$



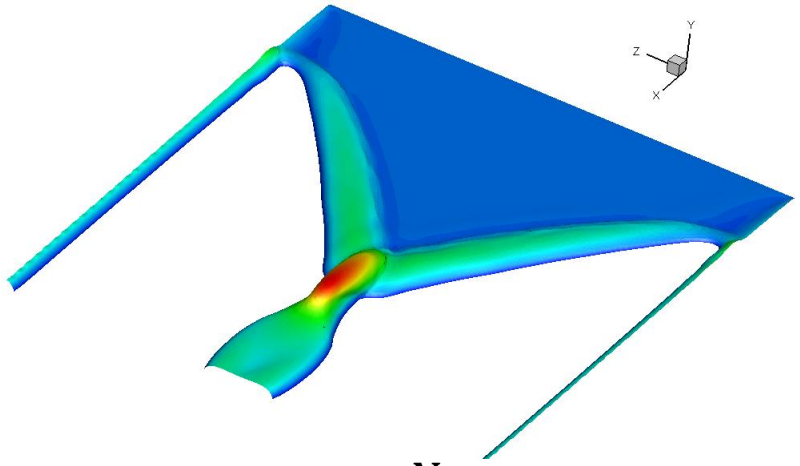
0.2 $\left[\frac{N}{m}\right]$

Surface tension impact

Re = 100



$0.03\left[\frac{N}{m}\right]$



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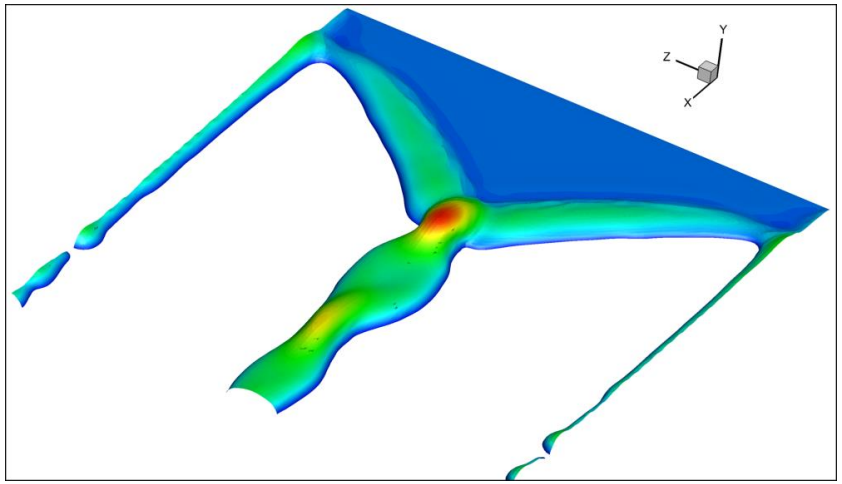
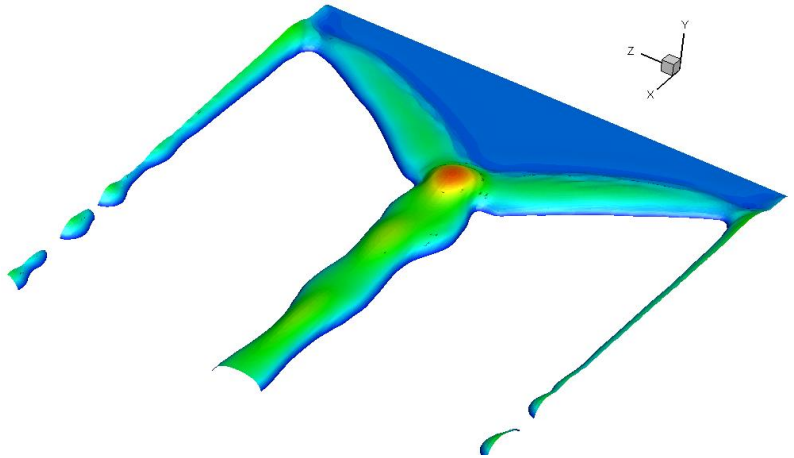
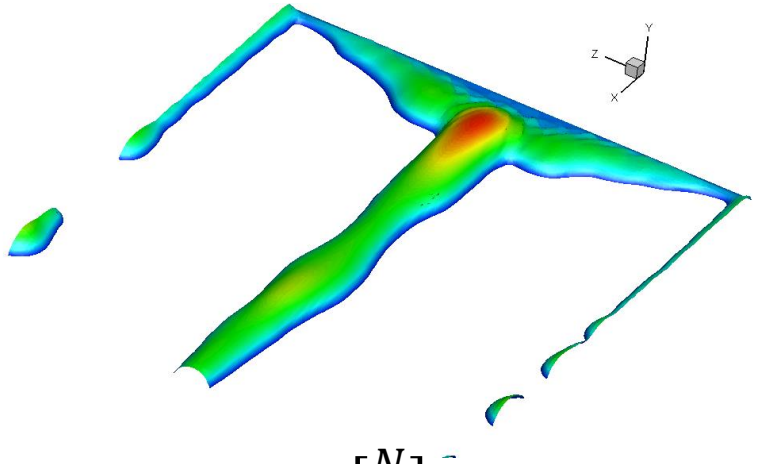


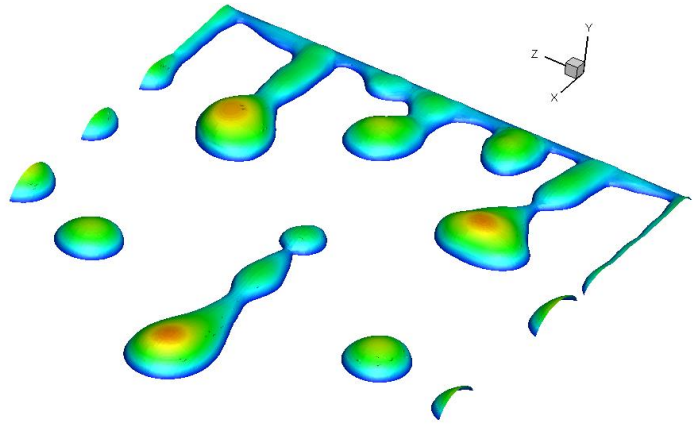
$0.07275\left[\frac{N}{m}\right]$



$0.09\left[\frac{N}{m}\right]$



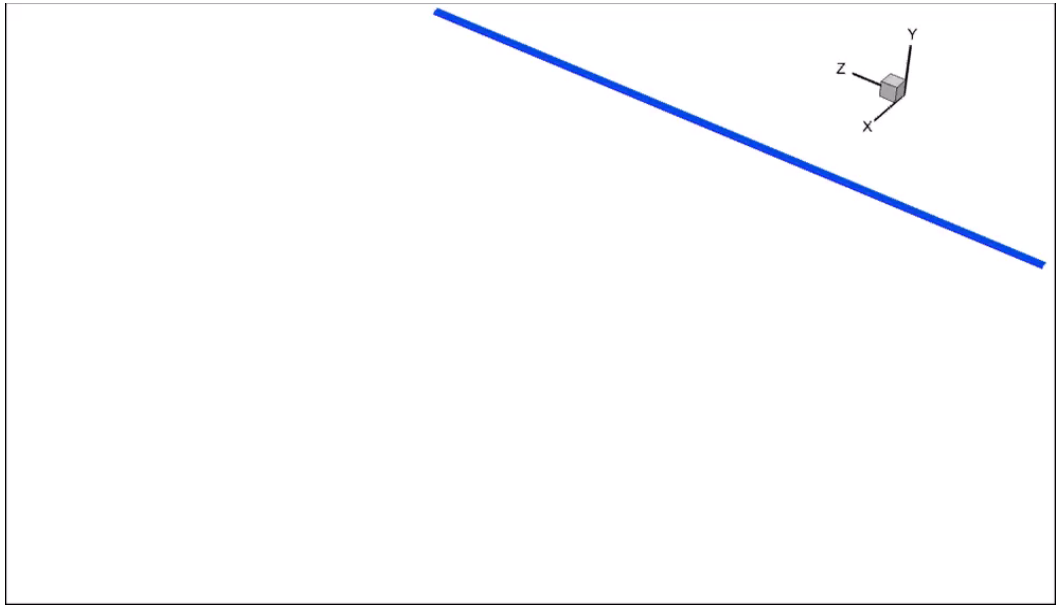
$0.14\left[\frac{N}{m}\right]$



$0.2\left[\frac{N}{m}\right]$

Summary

- numerical (CFD) model of liquid flow on a flat surface was developed
  - two phase unsteady Eulerian laminar flow, VOF, surface tension
  - creation of journal and UDF
  - need of multiprocessor machine ⇒ Cyfronet Pl-Grid Infrastructure
  - 3d model:
    - creation of model
    - mesh tests, time step tests, mesh strategy tests, initialization test
    - results dependent on Reynolds number: droplet, rivulet, film flow
    - reasonable flow picture & good agreement with available reference data
  - researched influence of:
    - contact angle
    - surface tension



Acknowledgements

The present research work was funded by the National Science Centre under the grant UMO-2014/15/B/ST8/04762.

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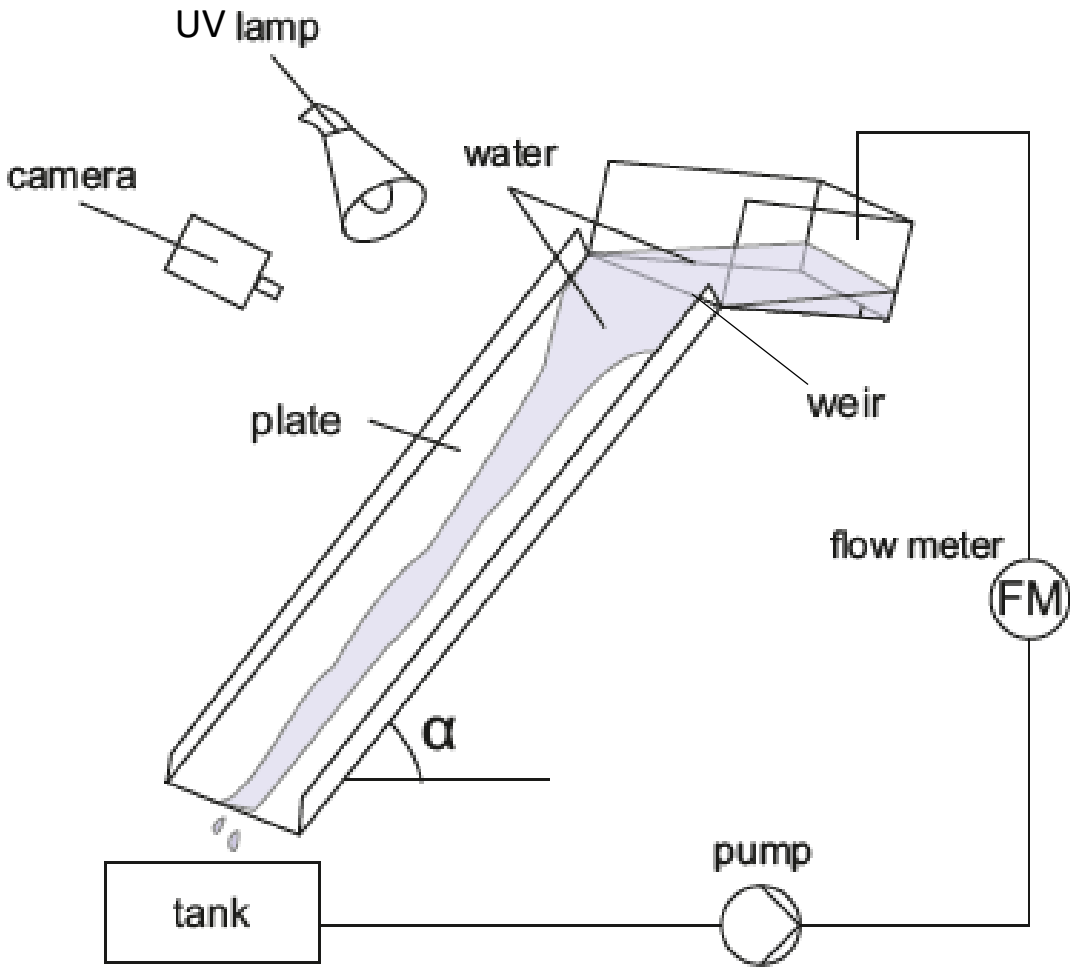
This research was supported by PL-Grid Infrastructure.

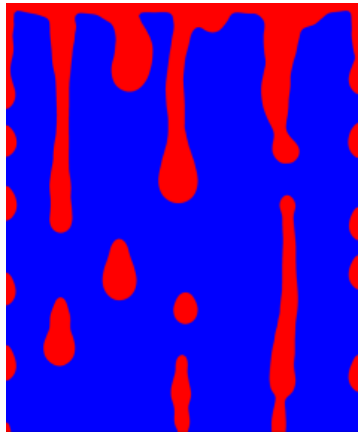
Thank you for your attention

Experiment

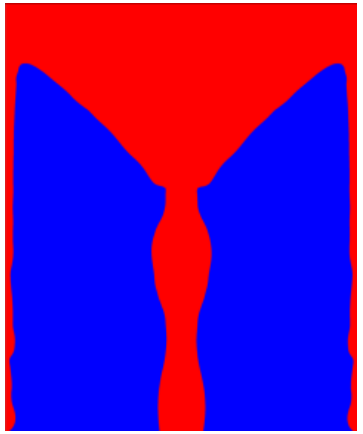


- coloured water by Rhodamine B
- sensitive to UV light
- closed system
- results are very sensitive to:
  - vibrations
  - room draft
  - micro surface irreularities

Comparison of experiment and simulation



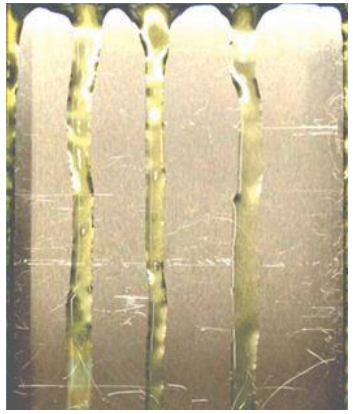
Re = 50



Re = 100

Re = 60

Re = 125



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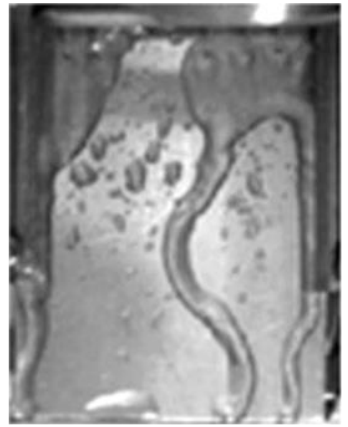

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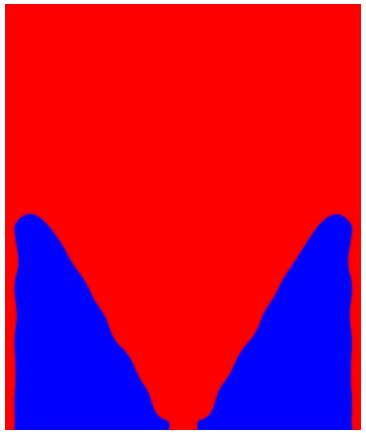

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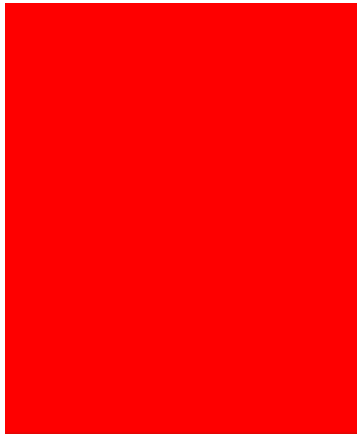

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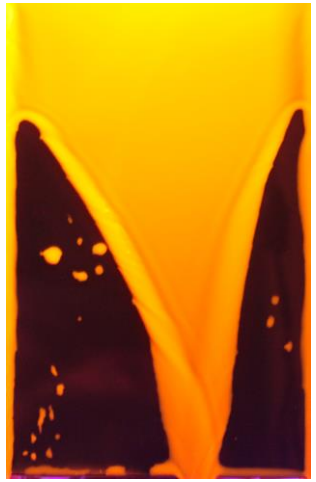

Re = 146

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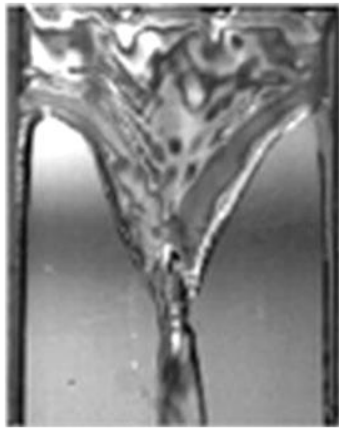

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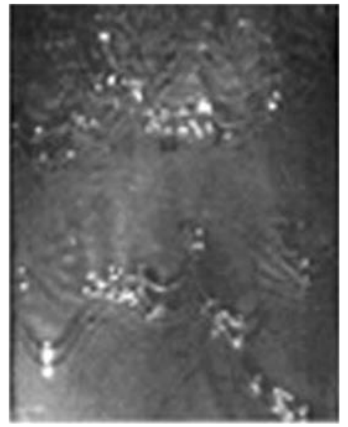
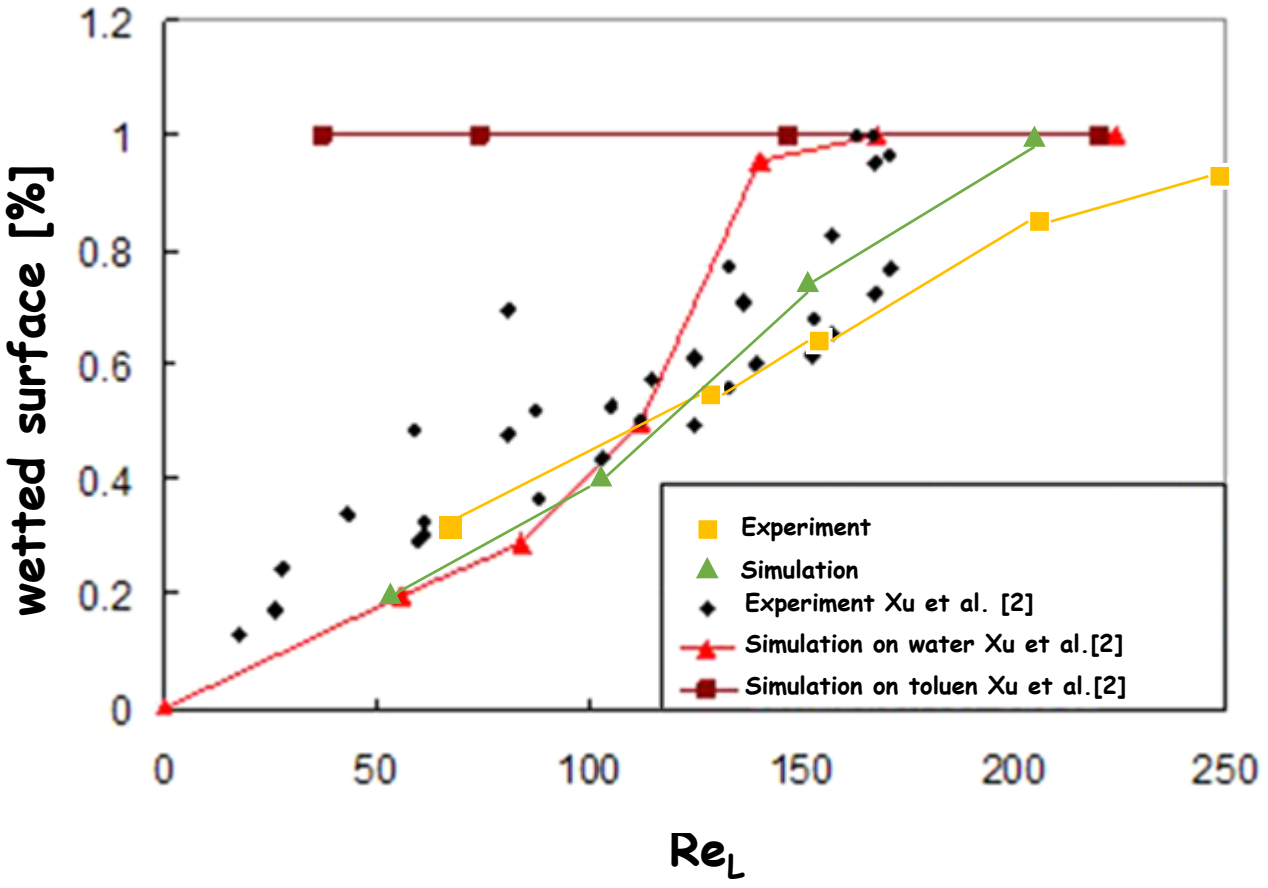


Re = 224 [2]

2) Xu Y. Y. et al. Ind. Eng. Chem. Res. 2014, vol. 53, p. 7797−7809

5) Iso Y. et al. Energy Procedia, 2013, 37, 860 – 868

Influence of Reynolds number



2) Xu Y. Y., Zhao M., Paschke S., Wozny, G.: "Detailed Investigations of the Countercurrent Multiphase (Gas−Liquid and Gas−Liquid−Liquid) Flow Behavior by Three-Dimensional Computational Fluid Dynamics Simulations", Ind. Eng. Chem. Res. 2014, vol. 53, p. 7797−7809