Numerical investigation of catalyst wetting inside trickle bed reactors

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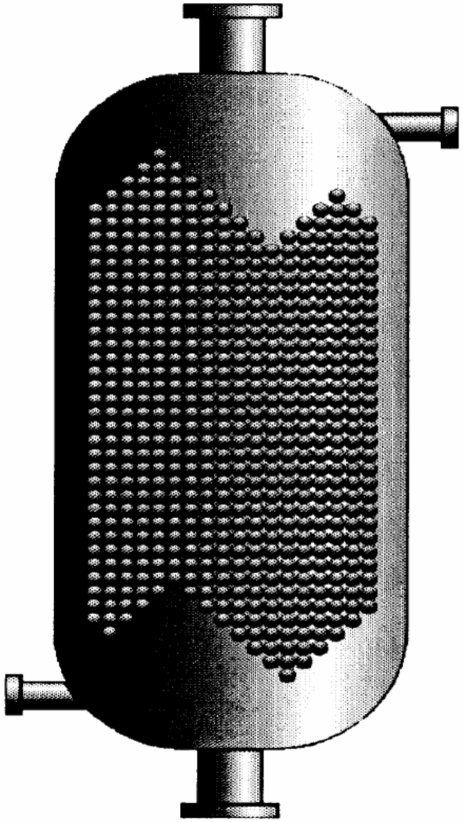
Plan

- **Introduction**
- **Problem of wetting in trickle bed reactors**
- **CFD modeling and results**
- **Short conclusion**

Fixed bed reactor

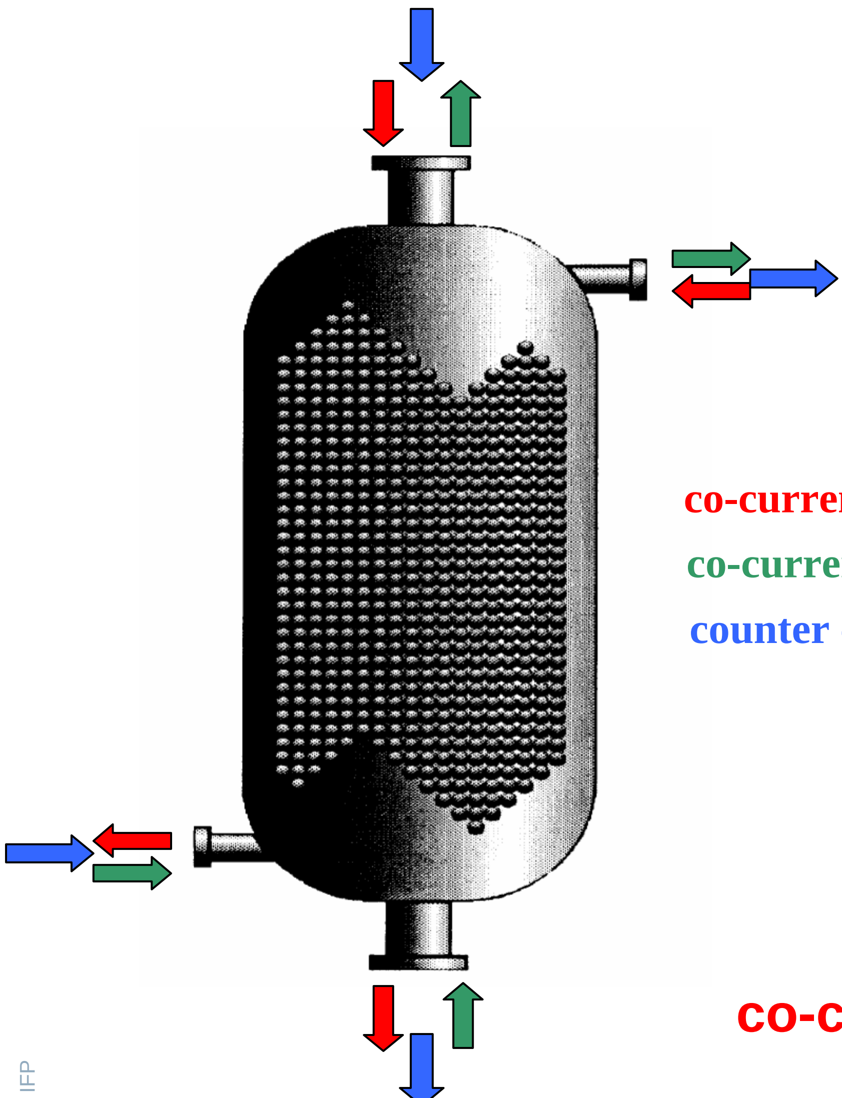


- Most common type of gas-liquid-solid reactors in the refining and petrochemical industries
- Simplicity; low operating costs associated
- Random packing or structured packing as solid catalyst
- Diameter = 1m to more than 5 m depending on the pressure

Fixed bed reactor : configuration and regime in two phase gas-liquid flow

Flow regimes

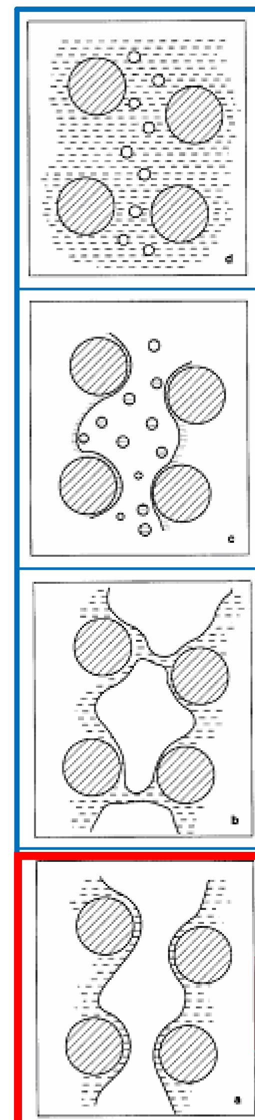
N. REINECKE. D. MEWES
Chemical Engineering Science. Vol. 51. No. 10. pp. 2131-2138. 1996



co-current downflow

co-current upflow

counter current



bubble flow

spray flow

pulse flow

trickle flow

co-current downflow

Trickle bed reactor in oil refining

- **Hydrotreatments of gasoils, atmospheric or void petroleum resids**
  - **Flow rates**

    industrial reactor : Vsl = 0.1 – 0.8 cm/s ; Vsg = 1 - 10 cm/s

    pilot reactor : Vsl = 0.01 – 0.08 cm/s ; Vsg = 0.1 - 1 cm/s
  - **Properties**

    $\rho_l = 700 - 900\ kg/m^3$. $\rho_g = 10 - 50\ kg/m^3$

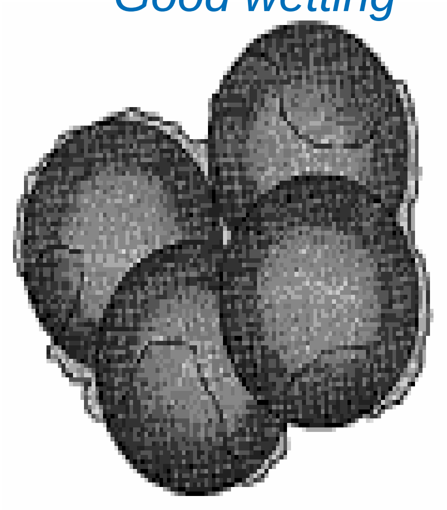
    $\mu_l = 0.5 – 1.5\ cP$

    $\sigma = 5 - 30\ mN/m$

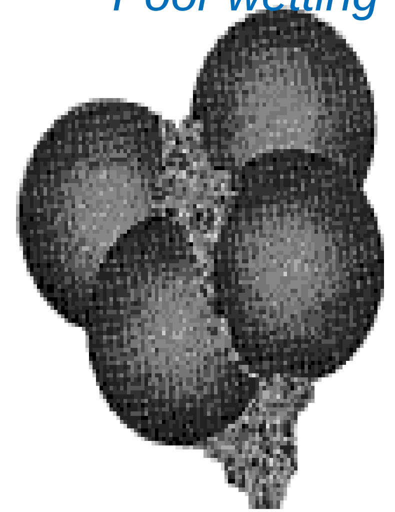
- **Pressure up to 200 bars**
- **Temperature up to 400 °C**

Wetting at the scale of the particle catalyst

Good wetting



Poor wetting



The effect is asserted by solving a reaction-diffusion equation inside catalyst particle

$$D_e \nabla^2 C = kC^n$$

Wet part of the surface $\quad C = C_0$

Dry part of the surface $\quad \frac{\partial C}{\partial n} = 0$

The effectiveness factor

$$\eta = \frac{1}{V_{cat}} \frac{\int kC^n \, dV}{kC_0^n}$$

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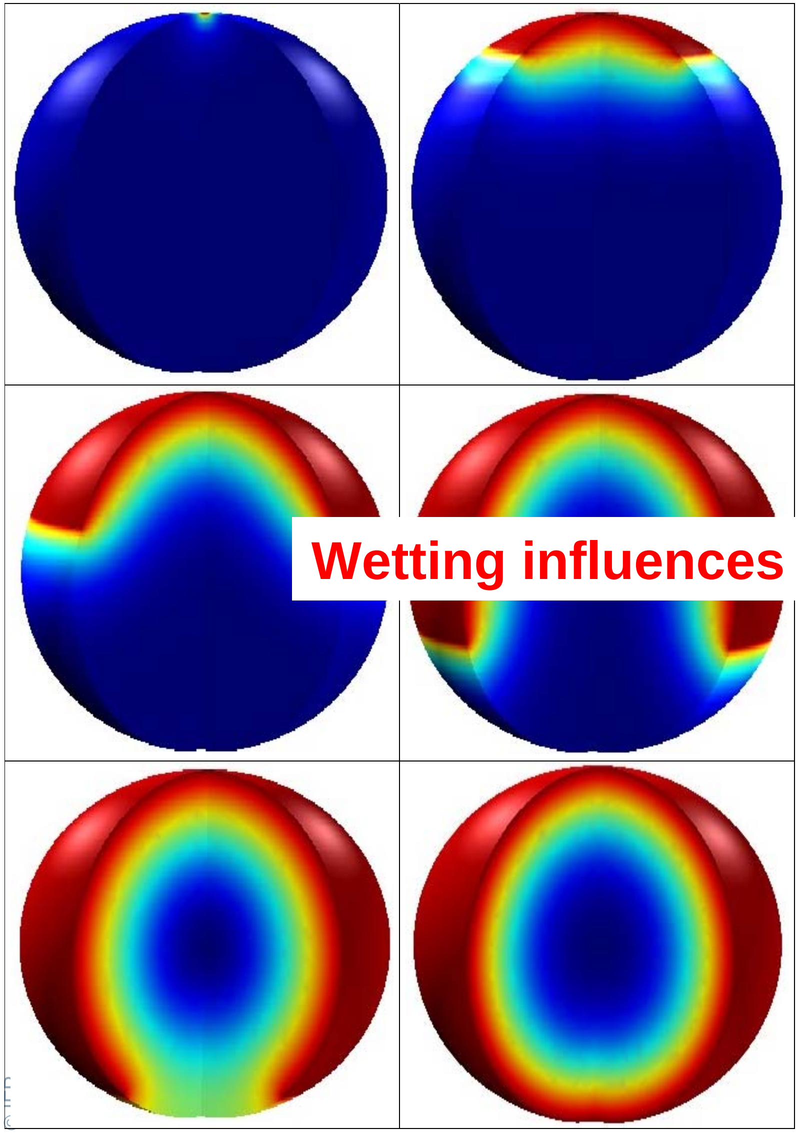
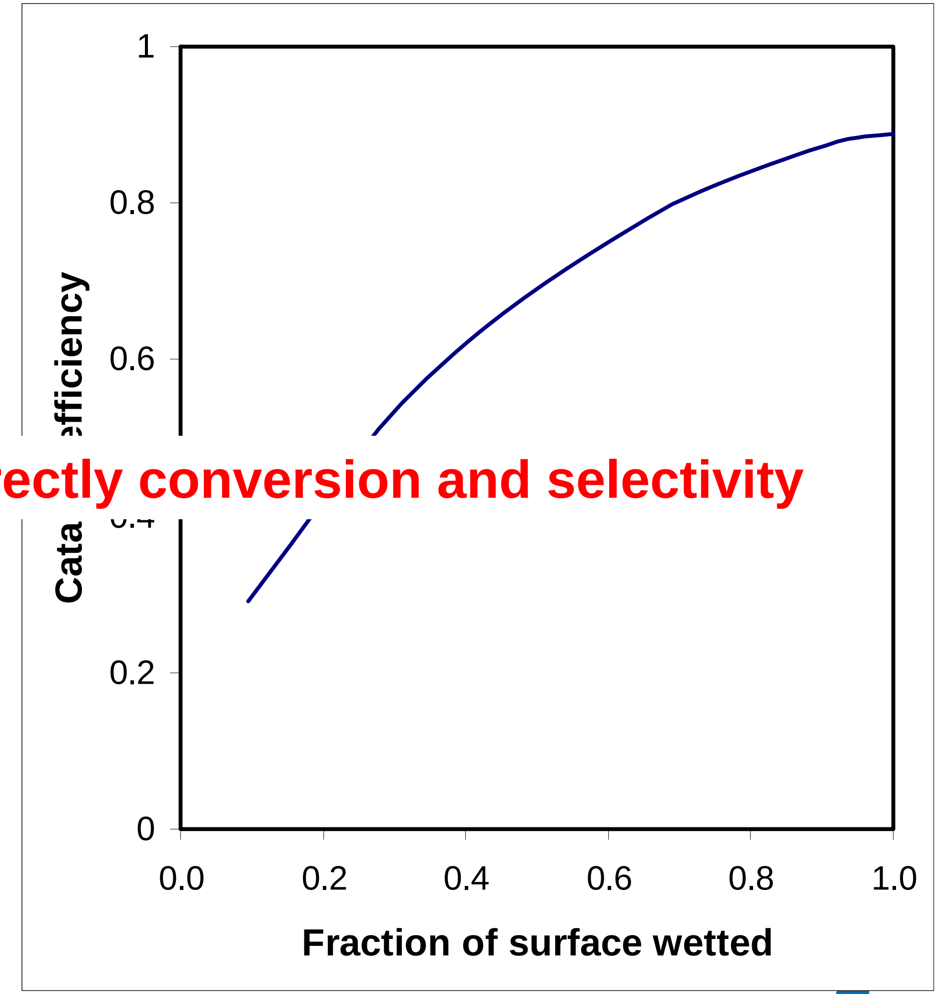
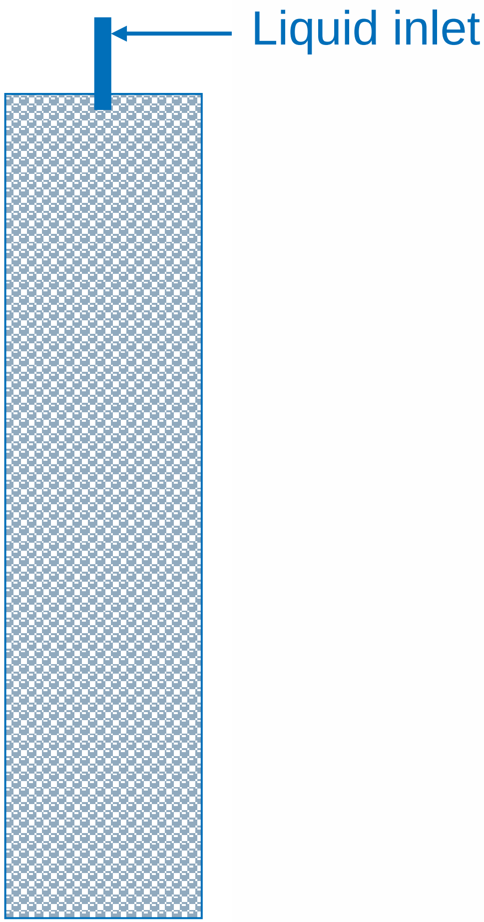
Consequences of a poor wetting

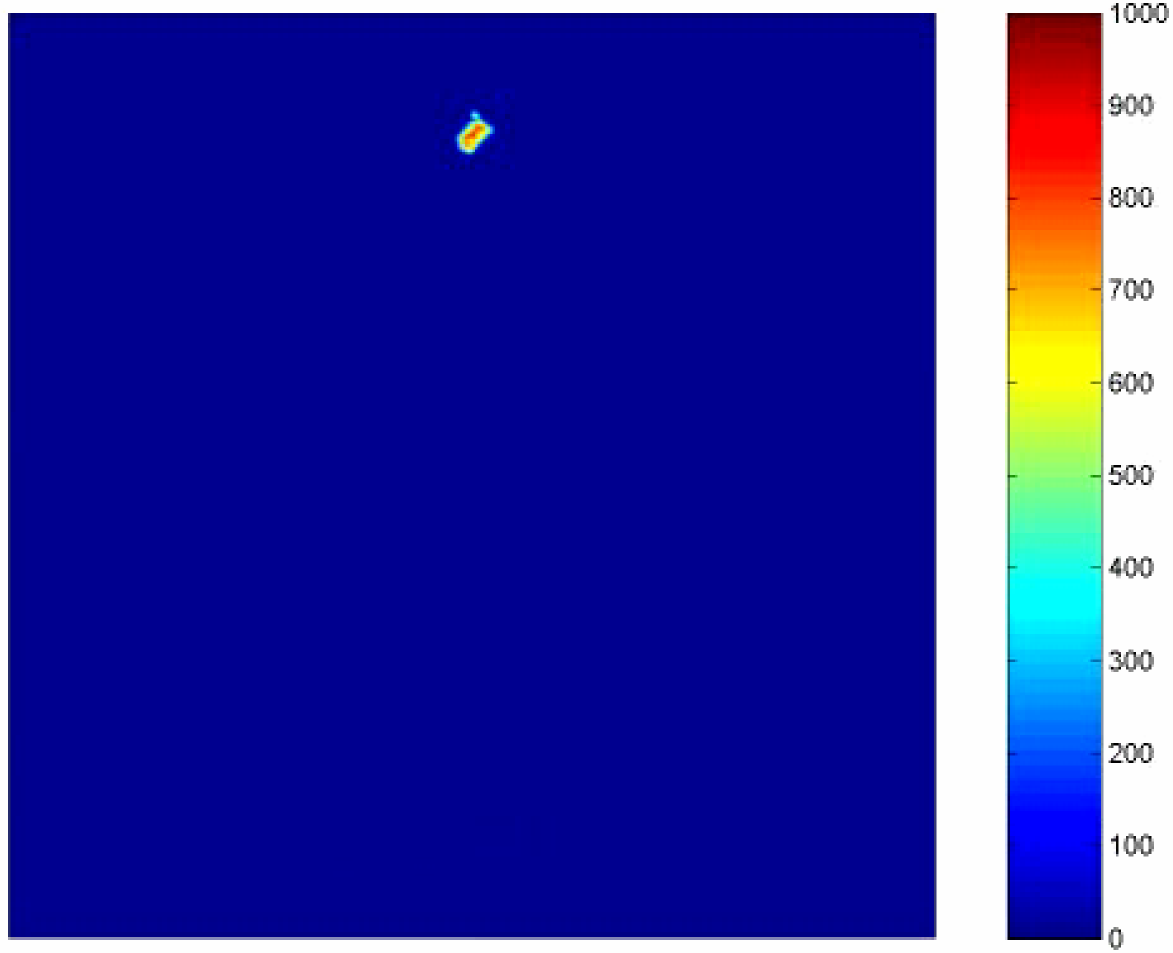




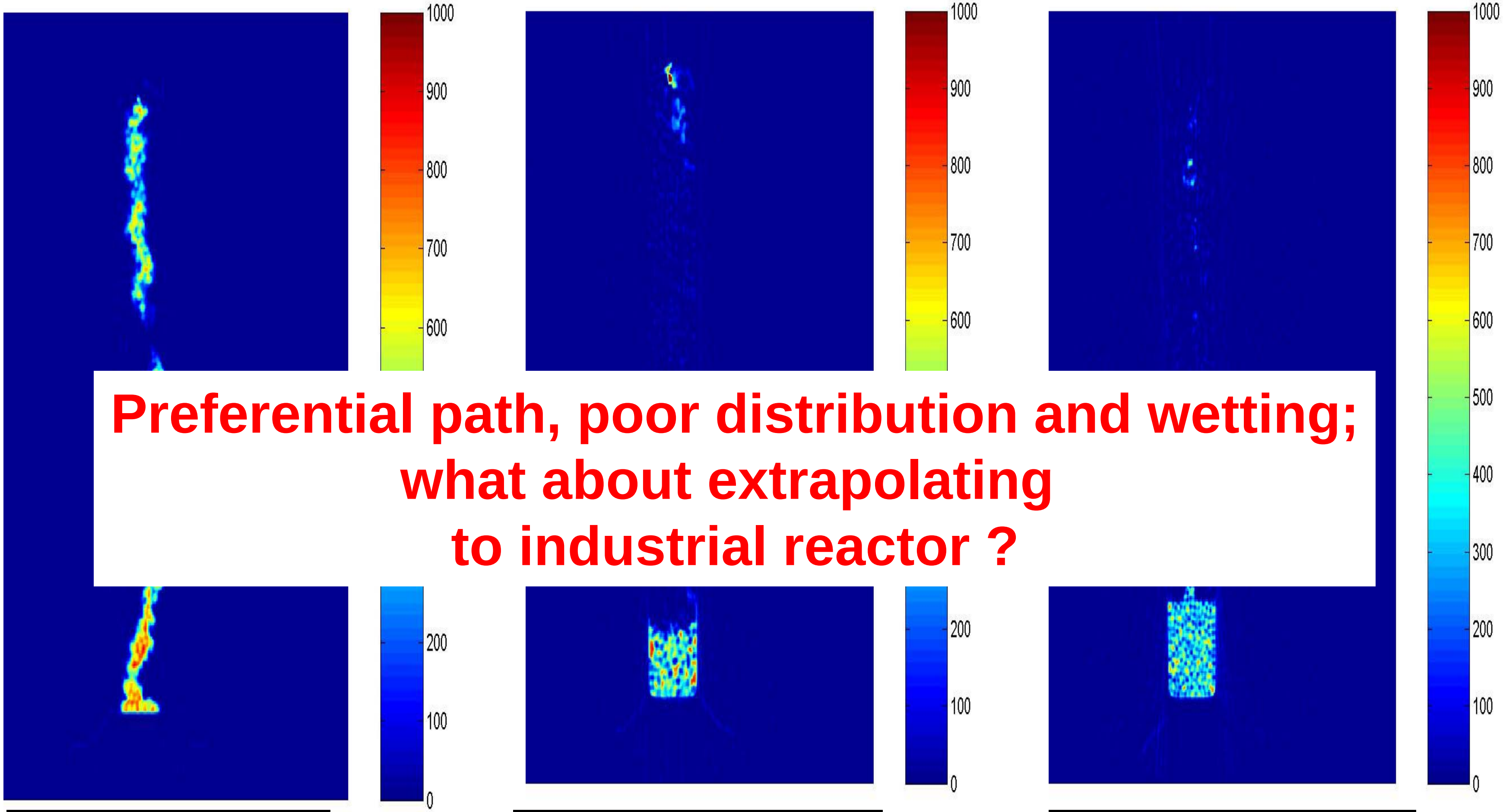
Wetting influences directly conversion and selectivity

Visualization of distribution and wetting using tomography at the scale of a pilot reactor





Tomography for different particles



Preferential path, poor distribution and wetting; what about extrapolating to industrial reactor ?

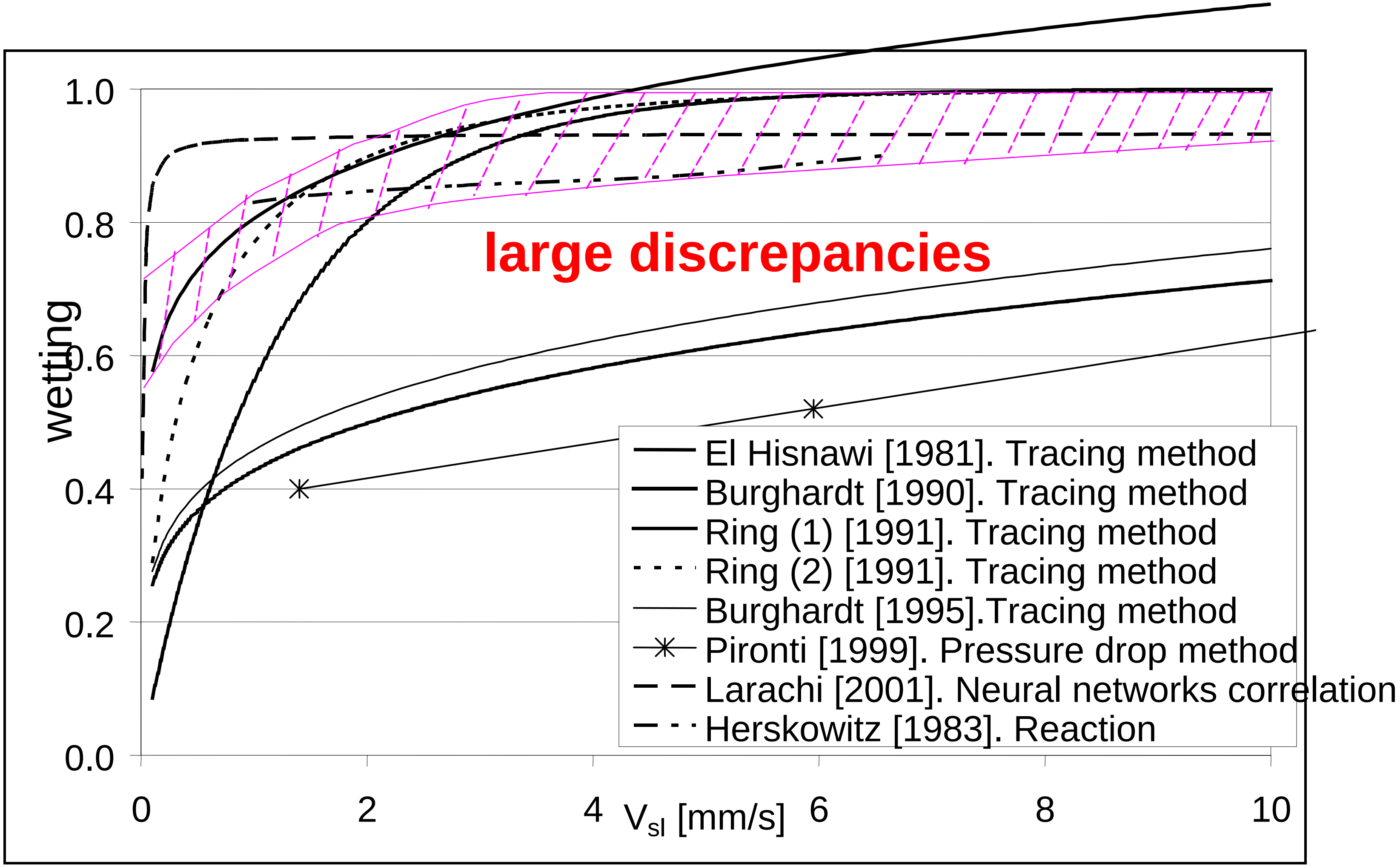
Alumina 2-4mm

Extrudates 2.6mm

Glass beads 2mm

Innovation Energie Environnement

Prediction of wetting : experimental investigations

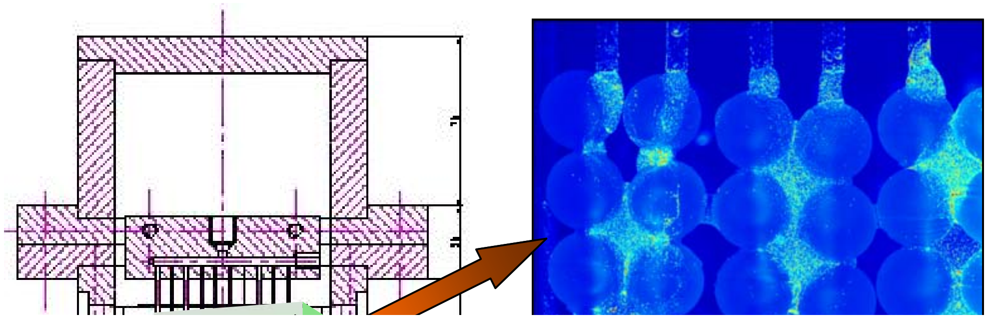


Experimental investigations at IFP

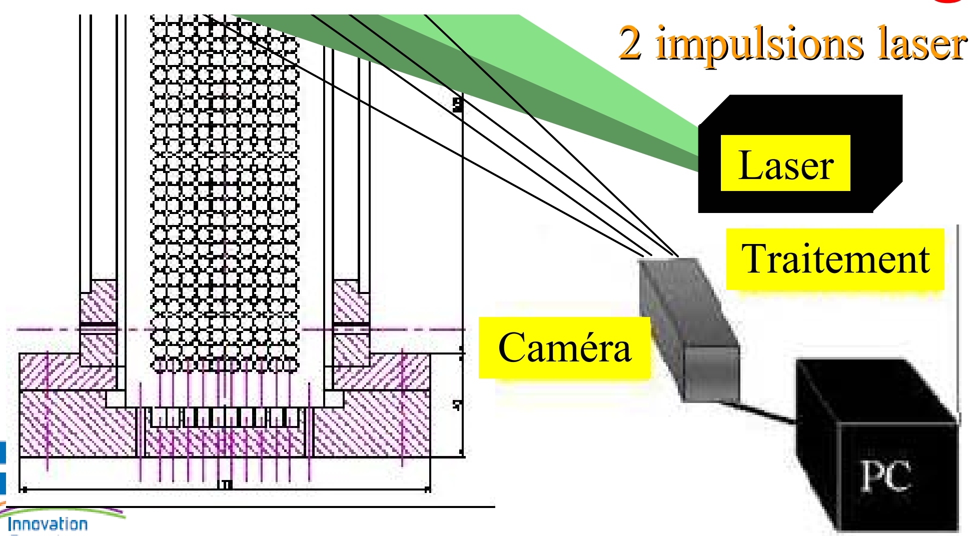
- **Parametric study of wetting in a particles bed**

  PIV method

L. Baussaron. PhD thesis. 2005



Situation to model using CFD



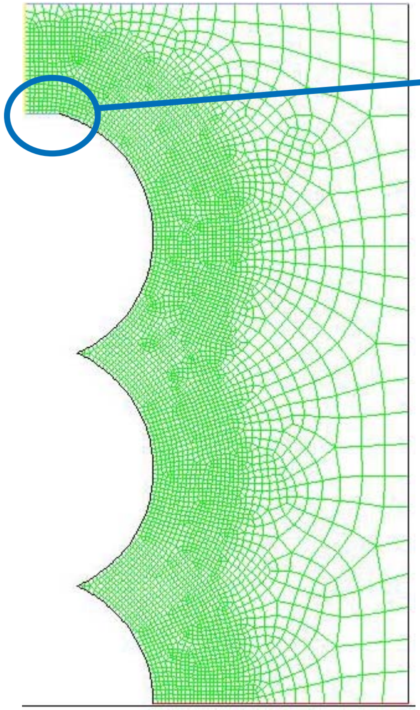
wetting

VOF model in Fluent 6.3 code

- **After a systematic study, algorithms and methods have been selected**
  - **Explicit Scheme**
    - **Non iterative Time Advancement**
    - **CICSAM algorithm for volume fraction equation**

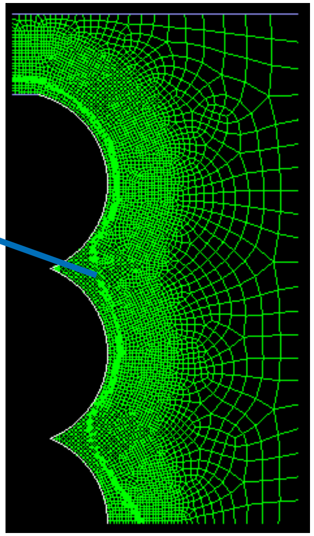
- **Brackbill model is used in Fluent 6.3 concerning wall adhesion force**

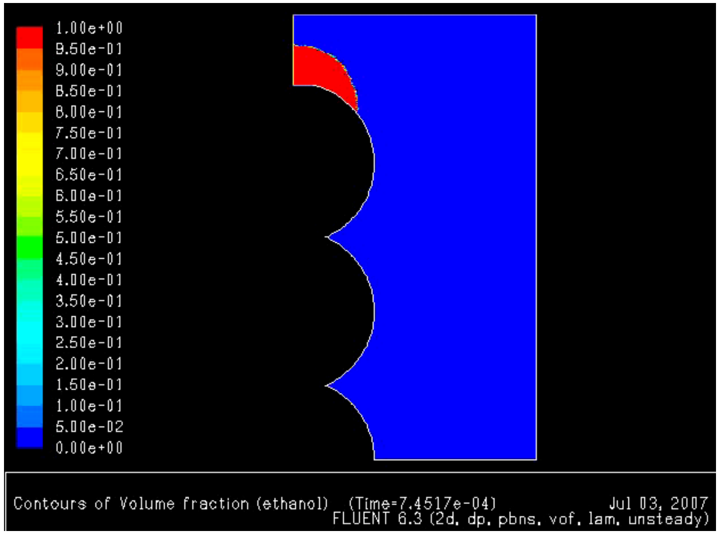
Mesh generation



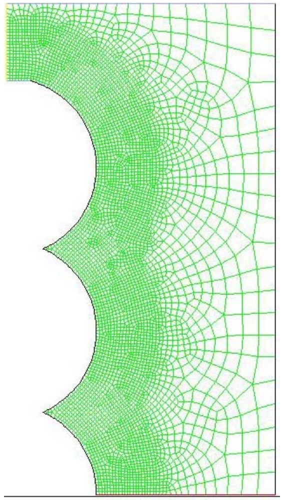
Special liquid inlet

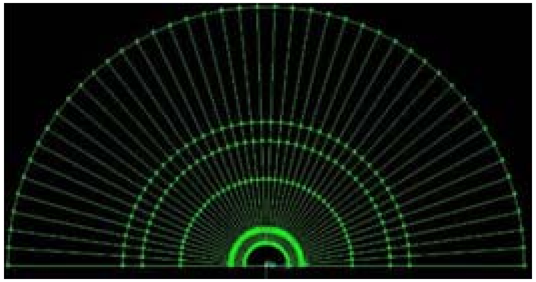
Mesh Adaption
with respect to void fraction

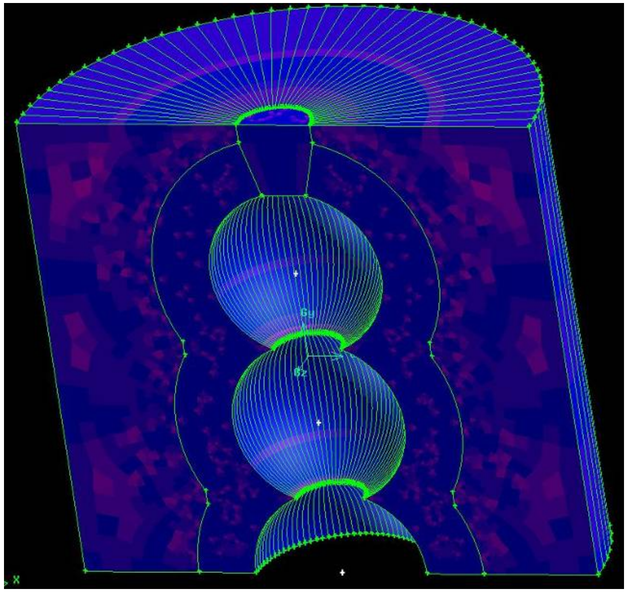




From 2D to 3D

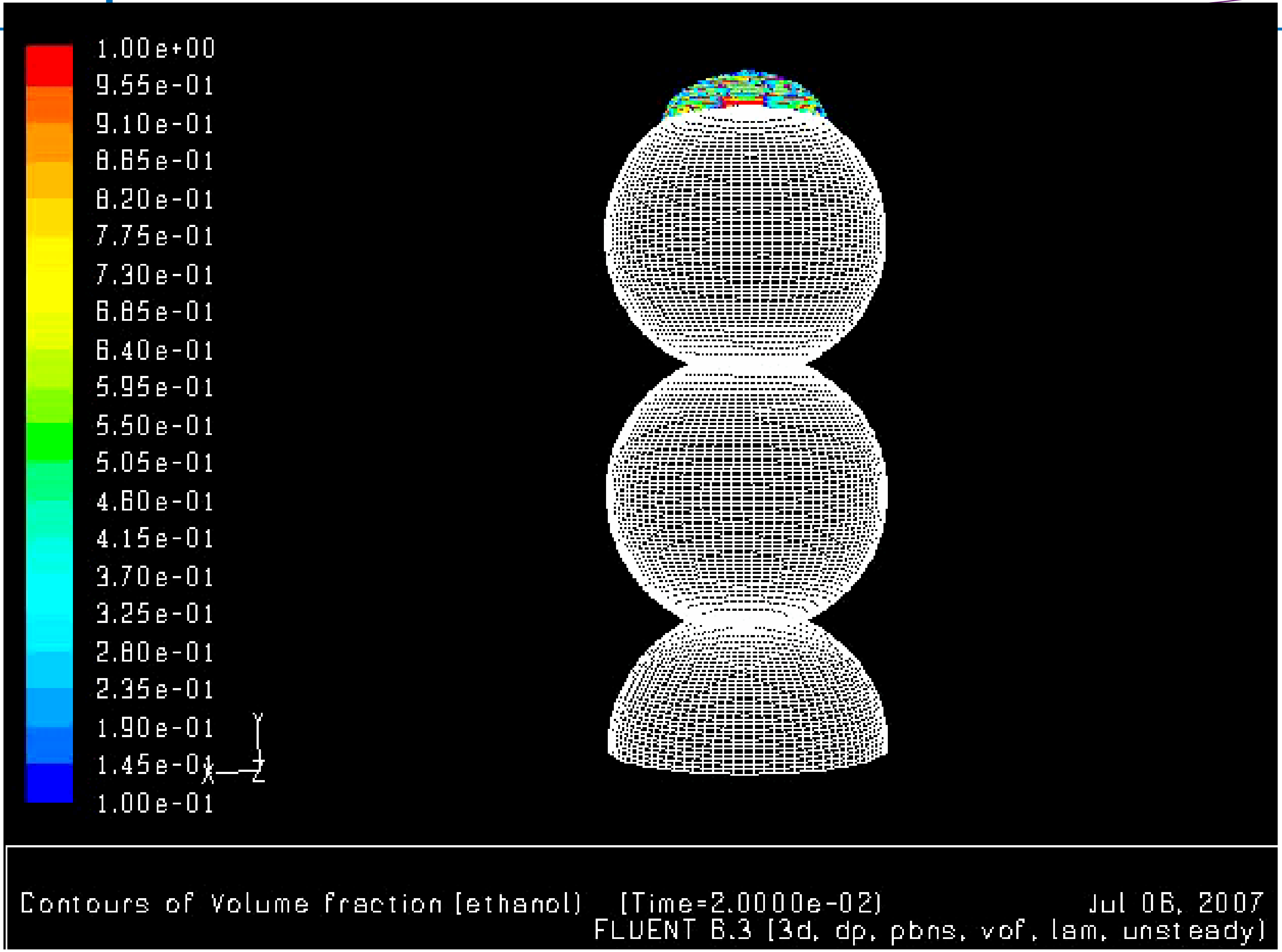






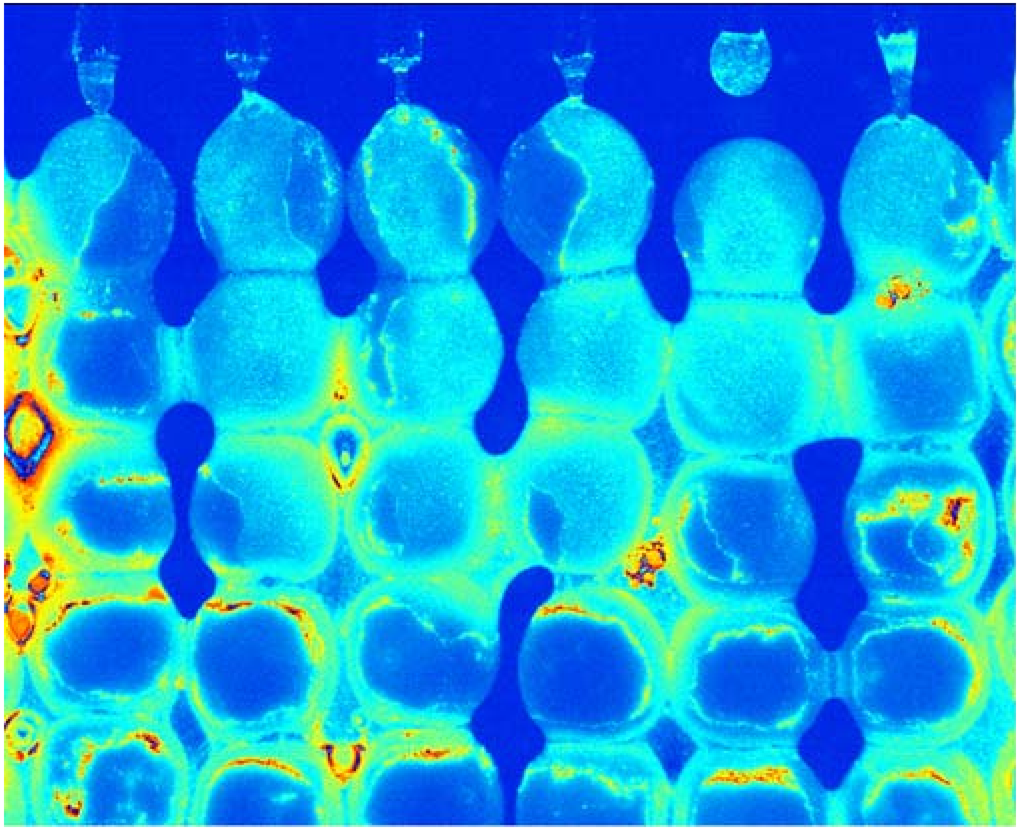
Few hundreds thousands cells

Example of a simulation result

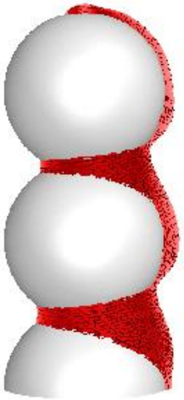


Physical behavior reproduced qualitatively

First qualitative comparison



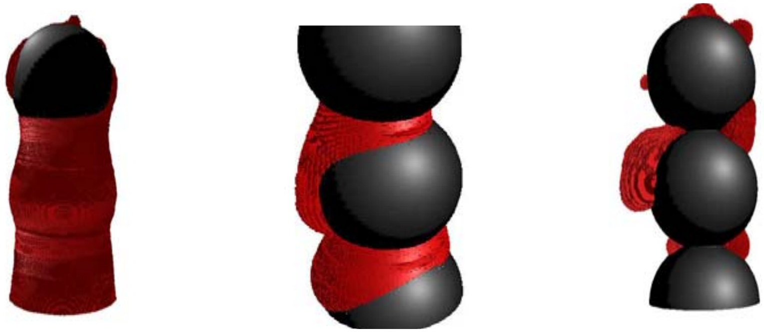
Experience



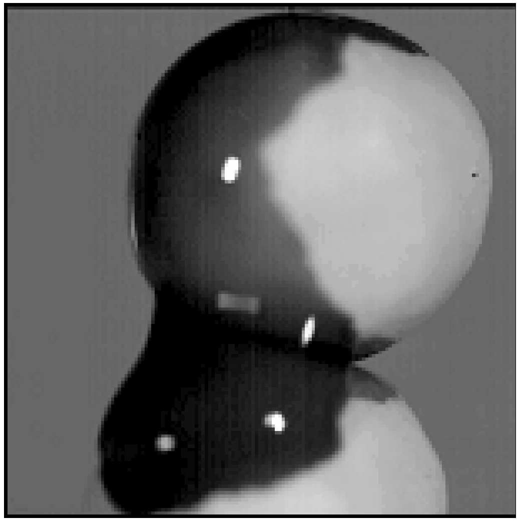
CFD

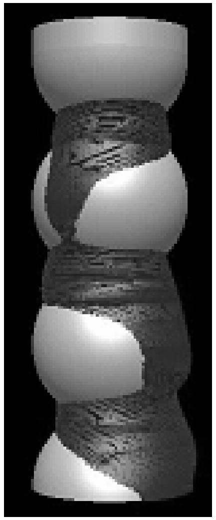
Results : flow regimes

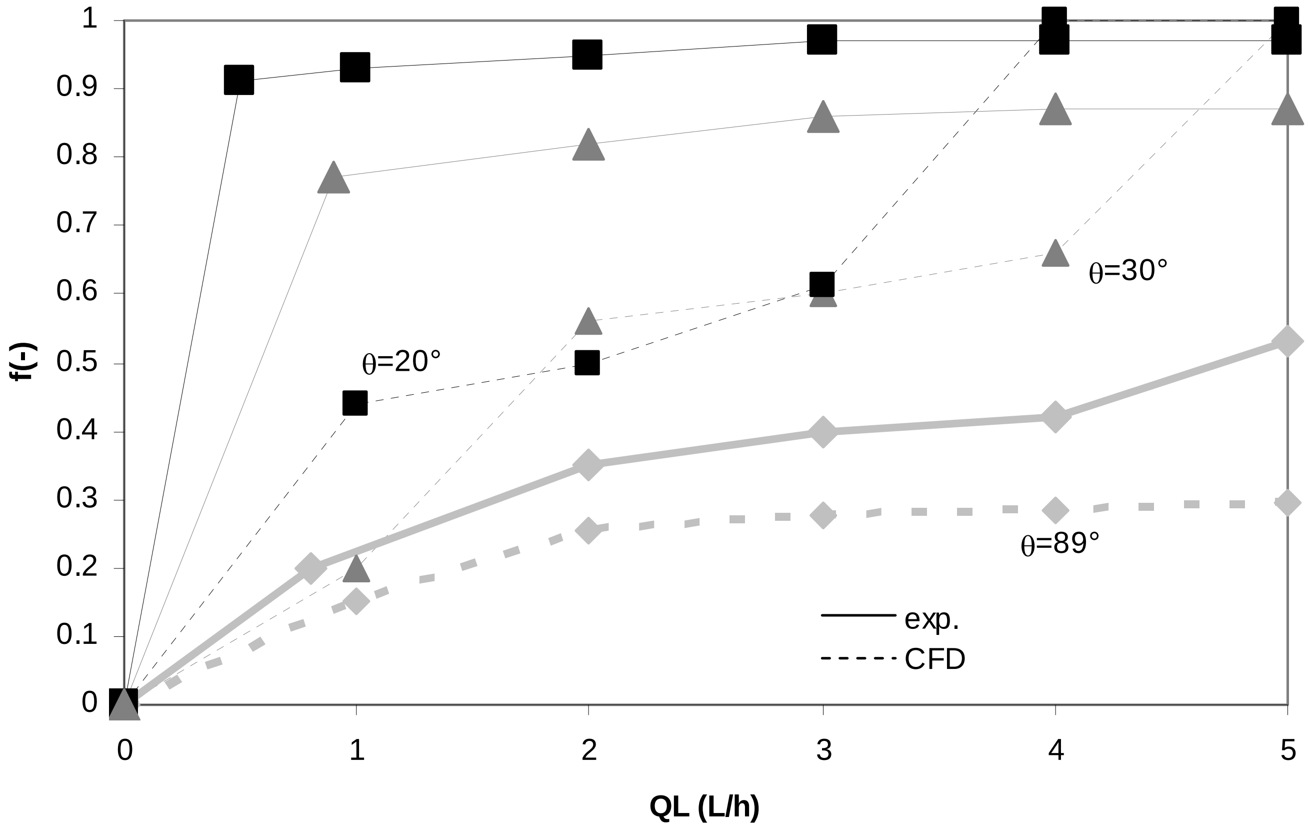
σ_s (mN/m)	Θ_c (°)	Q_l^* (l/h)	Flow regime
22	20	1 to 5	continuous film
22	30	2 to 5	
22	53	2 to 5	
22	53	1	film formation with rupture
73	20	1 to 4	growth and decrease of a single liquid volume
73	89	5	independent drops



Wetting fraction

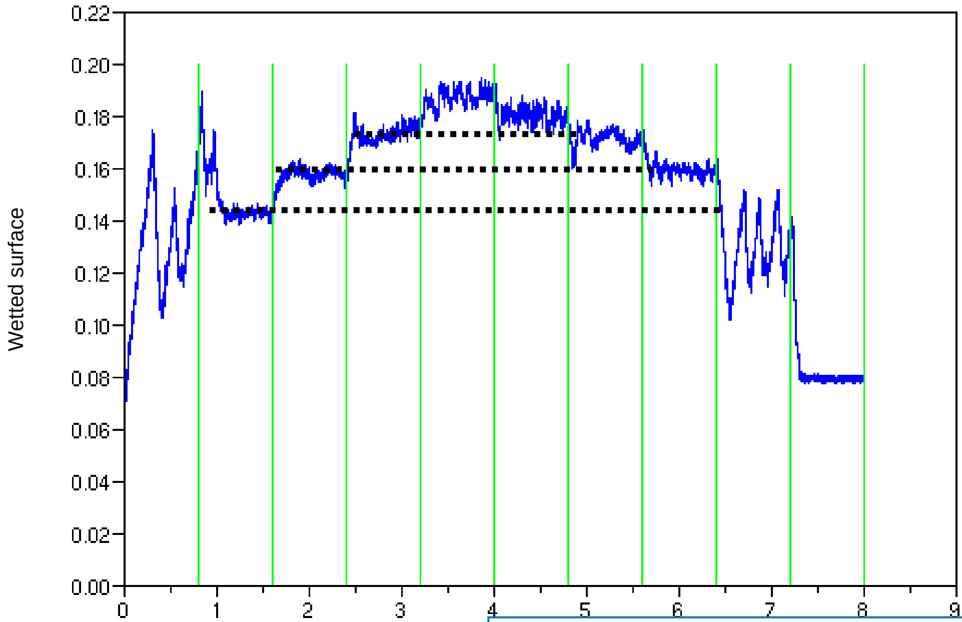




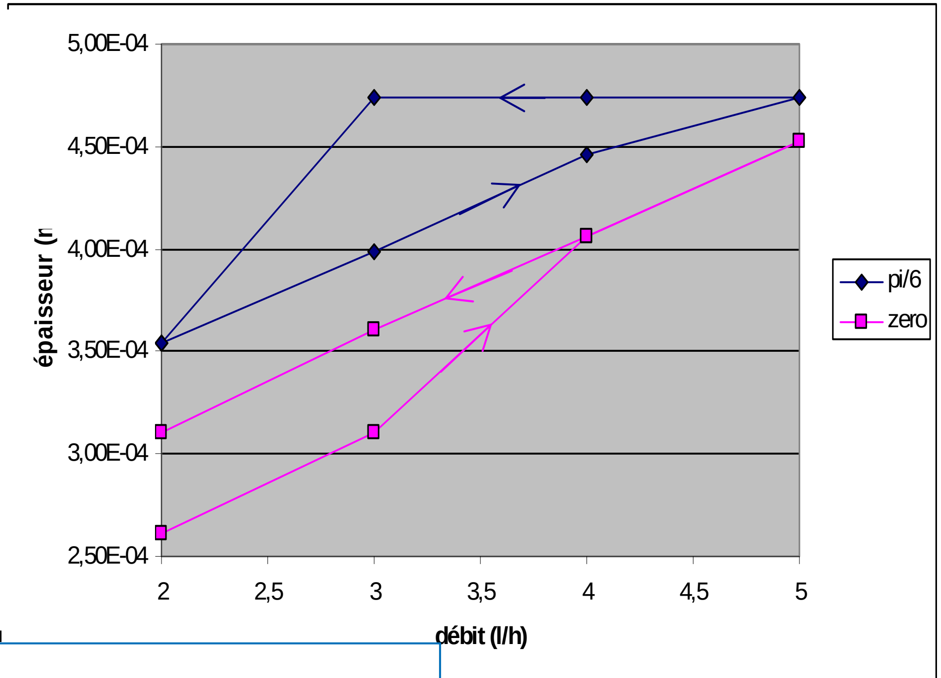


Wetting seems to be better predicted when the contact angle is high
Brackbill model correction ?

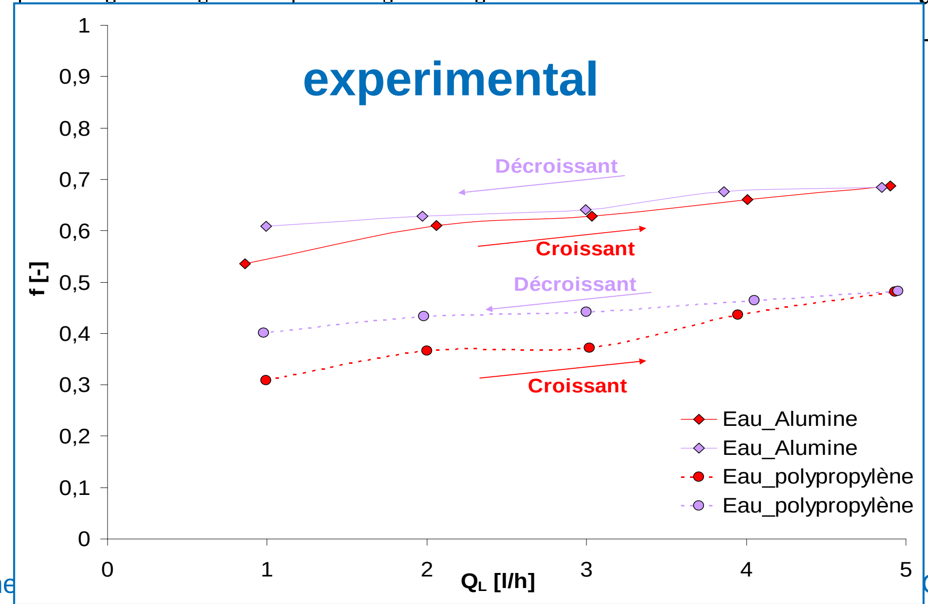
Hysteresis



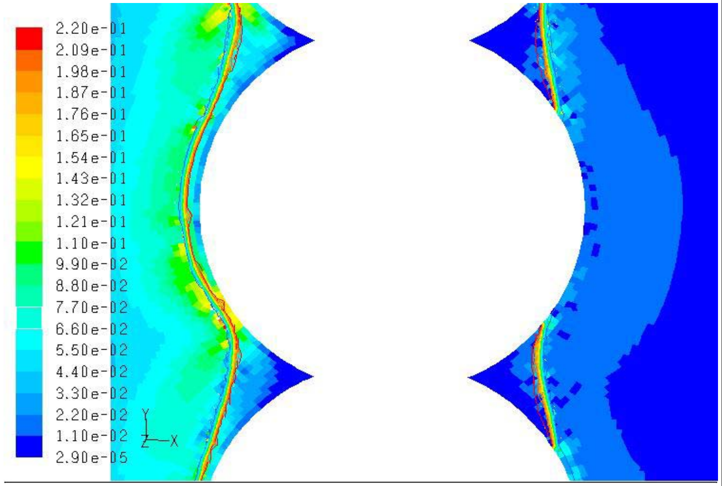
Wetted surface



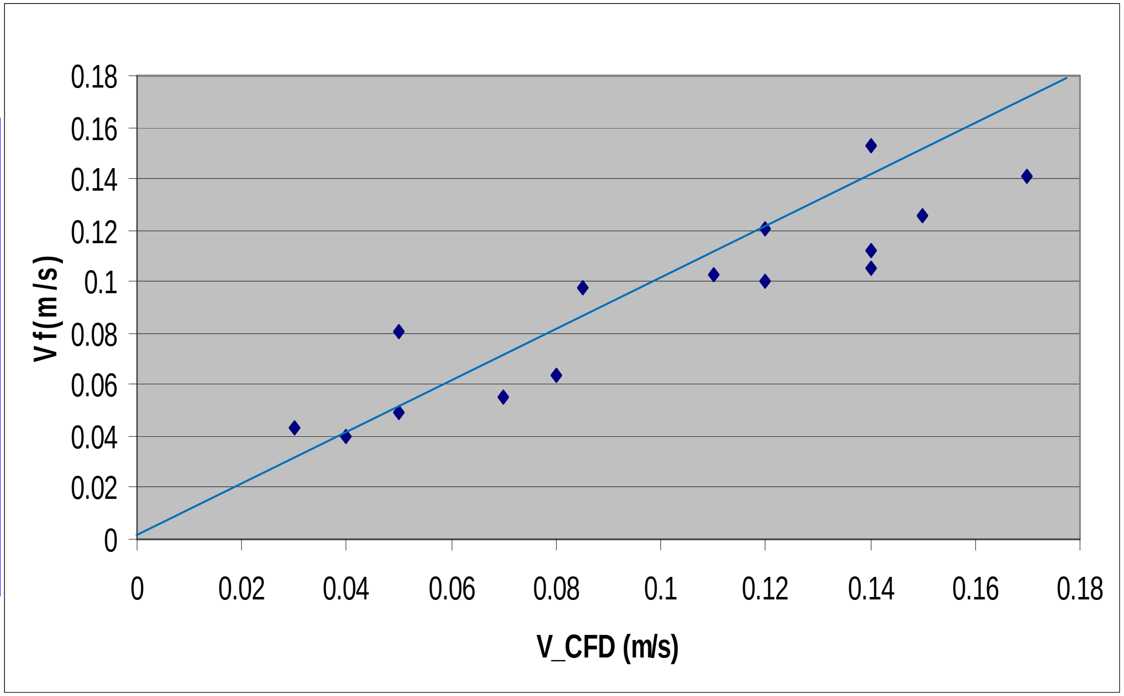
Film thickness



Film velocity



Velocity contours



Falling film theory:

$$V_f = \frac{\rho g \left(\frac{\delta}{2} \right)^2}{2\mu}$$

Quantitative results : static liquid holdup

Kramer. *Ch. Eng. Sci*. (1998)

contact angle (θ)	surface tension σ_s	CFD estimated static liquid holdup 2D	3D	correlation Charpentier
10	30	6.40%		3.53%
10	50	7.70%		4.00%
10	70	11.27%		4.24%
30	30	6.84%	8.33%	3.53%
30	50	10.60%	9.77%	4.00%
30	70	16.65%	11.57%	4.24%
50	30	12.47%		3.53%
50	50	11.19%		4.00%
50	70	4.05%		4.24%

Situation studied is less representative of a real fixed bed for which the correlation was build

Conclusion

- **In a simple situation :**
  - **VOF model gives qualitatively (and sometimes quantitatively) correct information concerning the wetting**
  - **For more quantitative results, one need better models concerning the expression of the interface force especially at the particle surface (contact angle)**