Hydrodynamics of Trickle Bed Reactors

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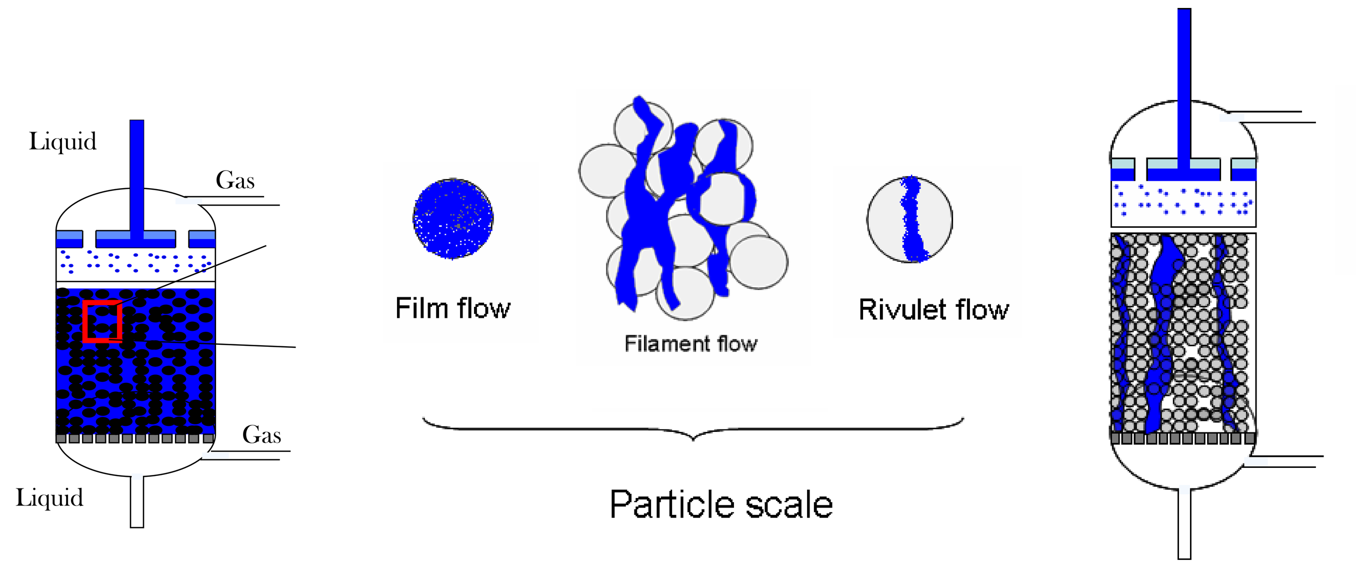
Introduction – trickle flow

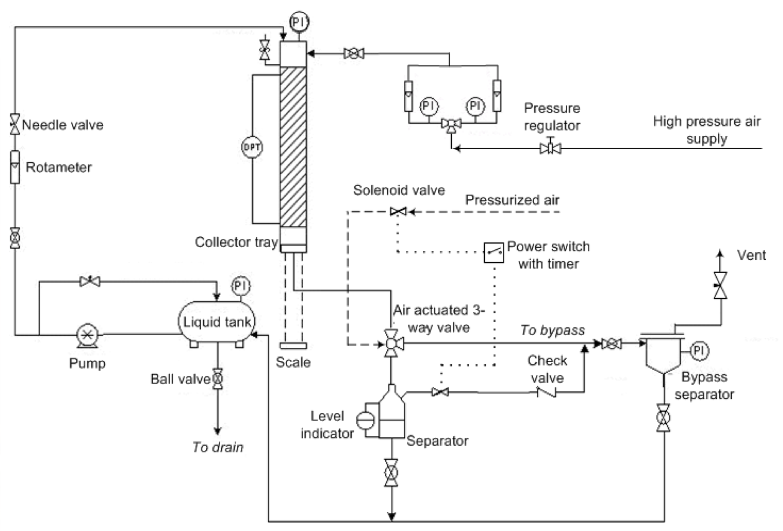


Focus of this work

- Experimental hydrodynamics investigation focused on the flow distribution
- Eulerian CFD modeling
- Development of validation methodology
- Extension of model – development of closures capable of capturing the effect of flow pattern

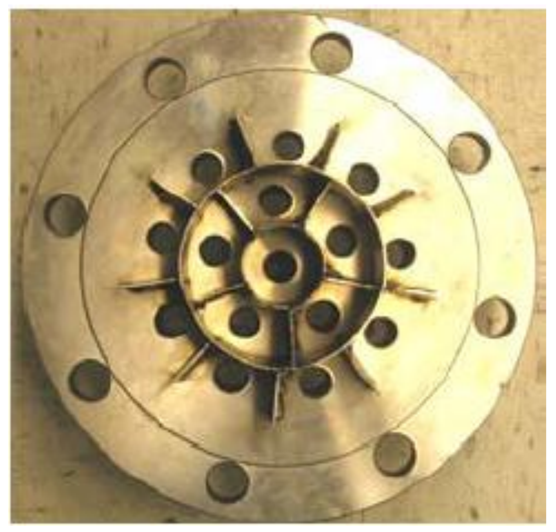
Experimental

High pressure trickle bed reactor



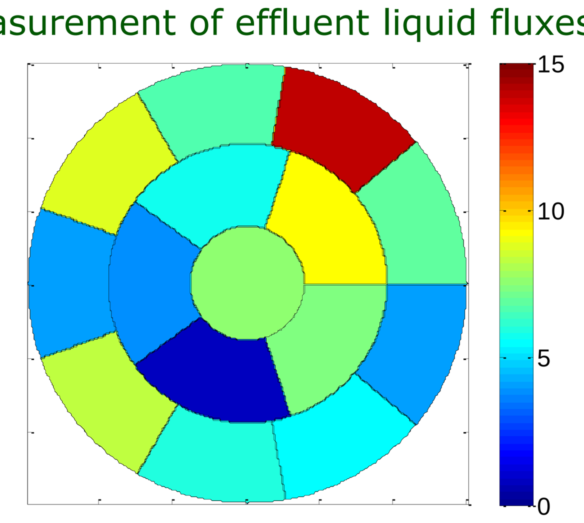
Experimental Conditions

Pressure, barg	1 to 8
Column Diameter, m	0.163
Bed Height, m	0.69
Fluids used	Water and Air
Packing	3 mm glass beads & 1.9 mm alumina extrudates

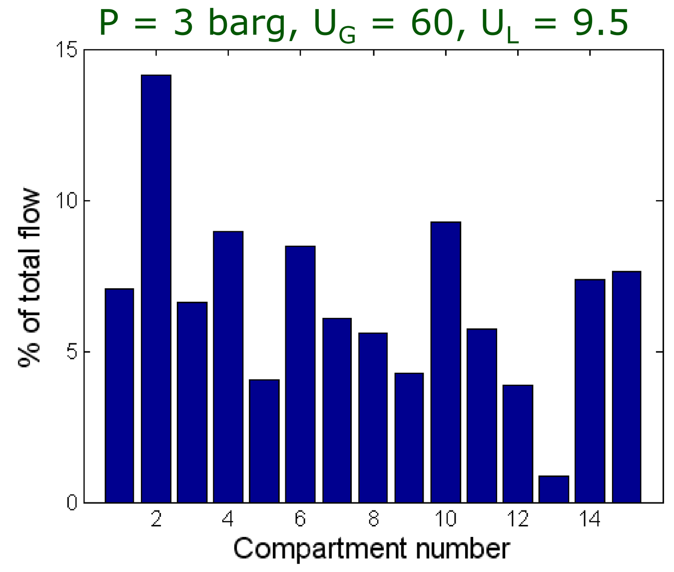


Collector used for fluxes measurements

Measurement of effluent liquid fluxes



P = 3 barg, U_G = 60, U_L = 9.5



Percentage of total flow in collector compartments

Characterization of the uniformity of liquid distribution

$$M_f = \sqrt{\frac{1}{N(N-1)}\sum_{i=1}^{N}\left(\frac{FLUX_i - \overline{FLUX}}{\overline{FLUX}}\right)^2}$$

N - Number of compartments (15)

$\overline{FLUX}$ - Average flux

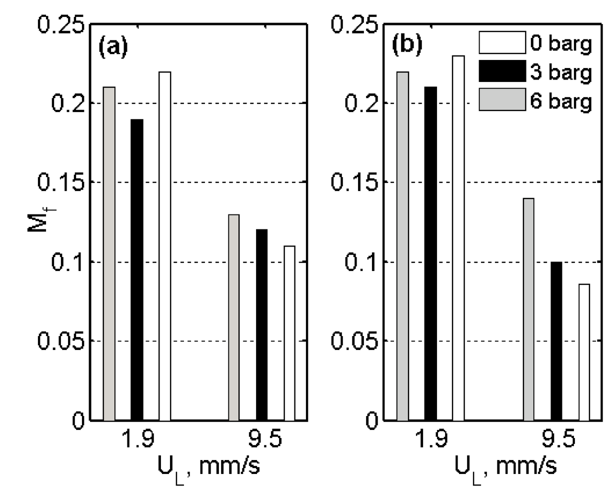
$FLUX_i$ - Flux in the compartment *i*

Maldistribution factor

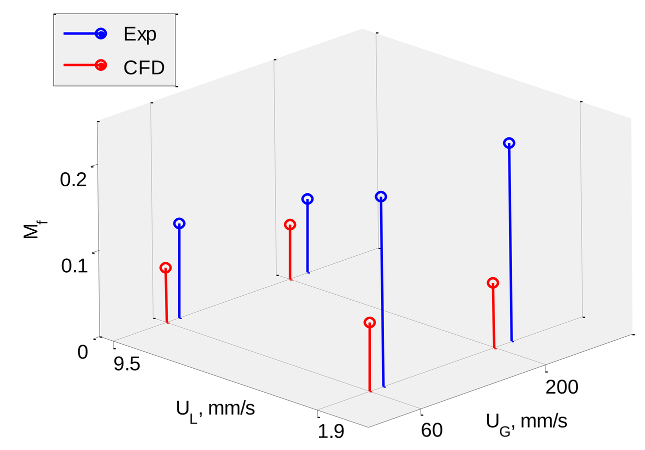
M_f = 0 - Uniform distribution

M_f = 1 - Completely maldistributed

- Most pronounced effect – liquid velocity
- Increased operating pressure or gas velocity do not significantly increase uniformity of liquid phase distribution

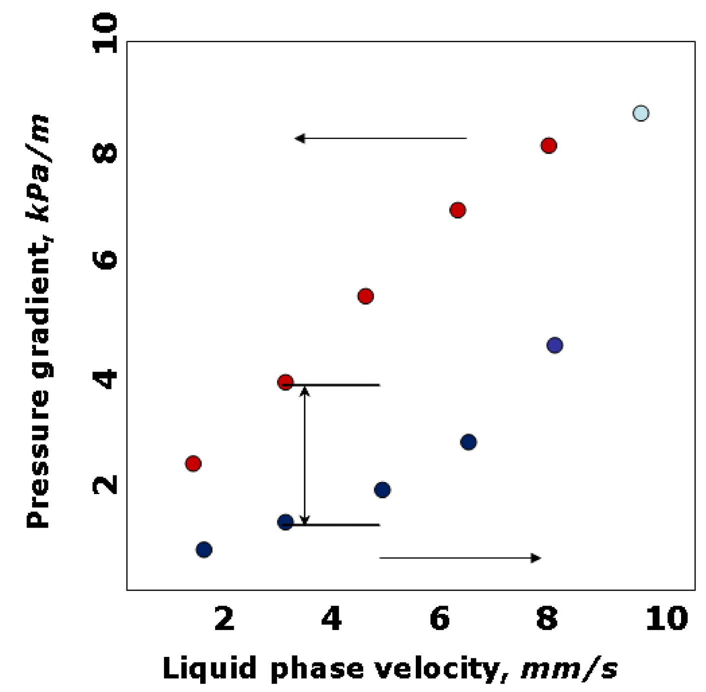


Maldistribution factor – experimental results



Comparison with CFD

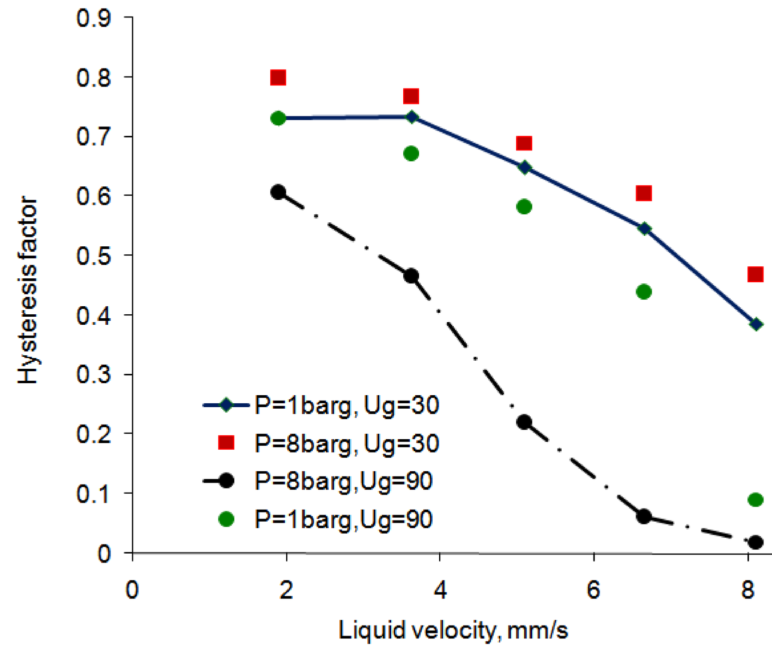
Hysteresis in trickle flow



$$f_H = 1 - \frac{(\Delta P/L)_{\text{Lower branch}}}{(\Delta P/L)_{\text{Upper branch}}}$$

f_H = 0 – no hysteresis

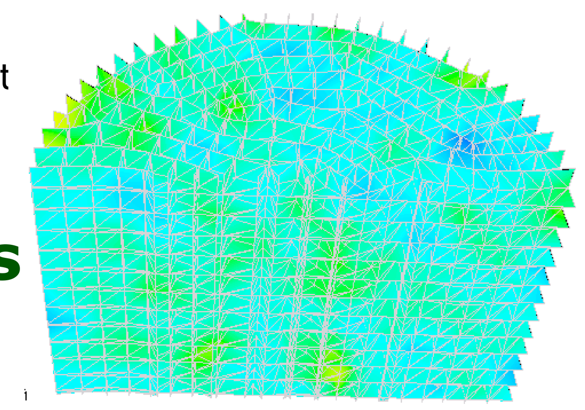
f_H - extent of hysteresis



Hysteresis factor – experimental results

- Dependence of the extent of hysteresis on the operating pressure is a strong function of the operating flowrates
- At the lower flowrates, hysteresis persists regardless of t pressure

Computational fluid dynamics modeling



Equations solved on the computational domain:

Conservation of mass

$$\frac{\partial \varepsilon_k \rho_k}{\partial t} + \nabla \cdot \varepsilon_k \rho_k \mathbf{u}_k = 0$$

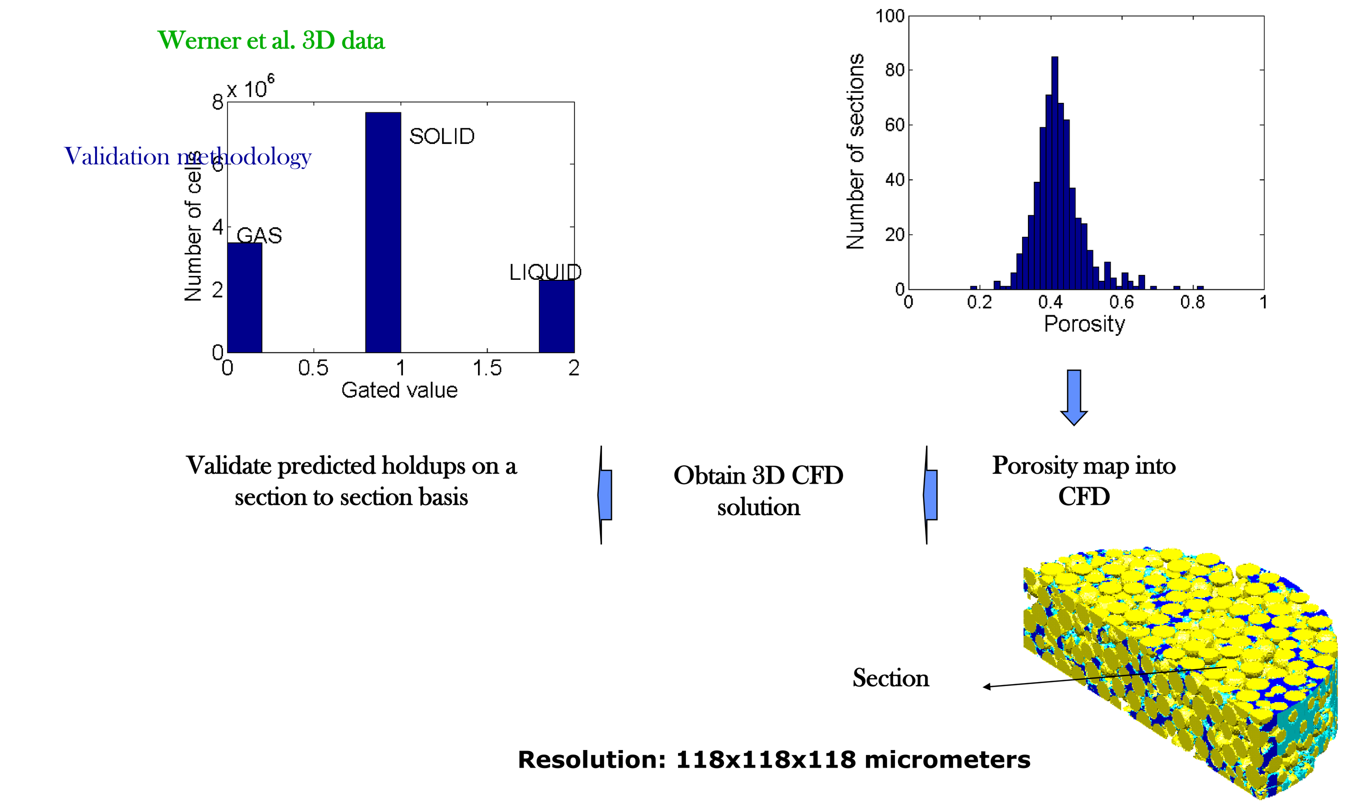
Conservation of momentum

$$\frac{\partial \varepsilon_k \rho_k \mathbf{u}_k}{\partial t} + \nabla \cdot \varepsilon_k \rho_k \mathbf{u}_k \mathbf{u}_k = -\varepsilon_k \nabla p + \nabla \cdot \varepsilon_k \mu_k \nabla \cdot \mathbf{u}_k + \sum_{q=1}^{nq} F_{k,q}(\mathbf{u}_k - \mathbf{u}_q) + S$$

Need:

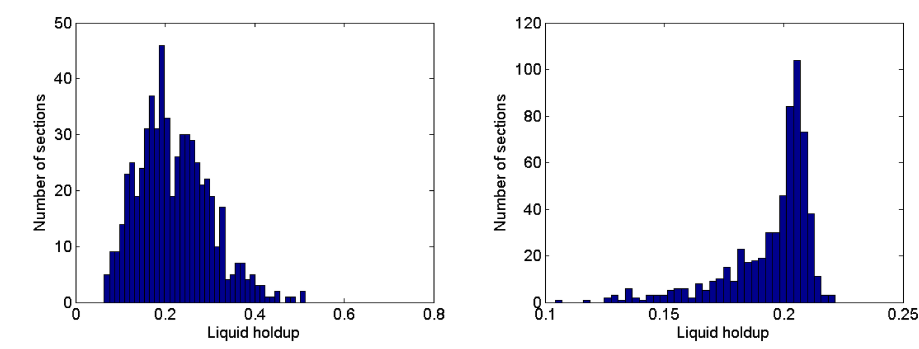
- Porosity distribution on the domain – Gaussian (Jiang et al., 2001)
- Phase interactions closures (Attou et al., 1999)
- Capillary closure (Grosser et al., 1988)
- Solution strategy, Boundary and Initial Conditions

Computational Fluid Dynamics Modeling (Continued)



Resolution: 118x118x118 micrometers

Comparison with experiments



Conditions: Air-water-2.5 mm glass beads; atmospheric pressure; U_L=5.3 mm/s, U_G = 13 mm/s

Average error = 31.8%

Extension to account for flow structures other then film flow

$$Re_{min} = \frac{1}{E_1}\left(\frac{\varepsilon}{0.5}\right)^3 (1-\cos\theta)^3 Ga_L{}^3 \frac{\Delta P/\Delta z + \rho_L g}{\rho_L g}$$

(Wijffels et al. 1974)

E_1 - Ergun constant

ε - Bed porosity (volume fraction of voids)

θ - Contact angle

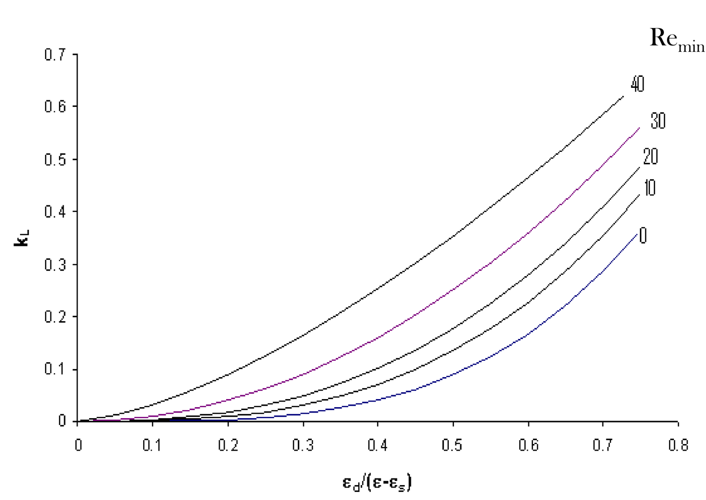
$$Ga_L = \frac{d_p{}^3 \rho_G{}^2 g}{\mu_G{}^2}$$ - Galileo number for liquid phase

Relative permeability model (Saez and Carbonell, 1985)

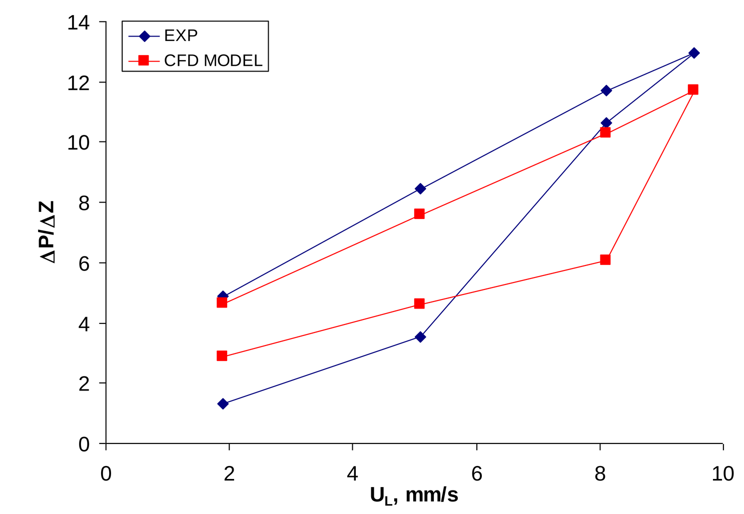
$$\left(-\frac{\Delta P}{\Delta z}\right)_{\text{two phase flow}} = \frac{\left(-\frac{\Delta P}{\Delta z}\right)_{\text{one phase flow}}}{k_L}$$

Rivulet flow

Film flow



Relative permeability as a function of wetting preferentiality (Crine et al. ,1992)



Prediction of hysteresis

Acknowledgements

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- TOTAL