8th International Berlin Workshop (IBW 8) on
Transport Phenomena with Moving Boundaries
25th - 26th October 2018, Berlin, Germany

Drop-based modelling of coalescence in batch settlers including polydispersity

David Leleu, Andreas Pfennig
andreas.pfennig@uliege.be
Products, Environment, and Processes (PEPs)
Department of Chemical Engineering
Université de Liège
www.chemeng.uliege.be/Pfennig

Supported by:
Federal Ministry for Economic Affairs and Energy
on the basis of a decision by the German Bundestag

PEPs CHEMICAL ENGINEERING

LIÈGE université 200

agenda

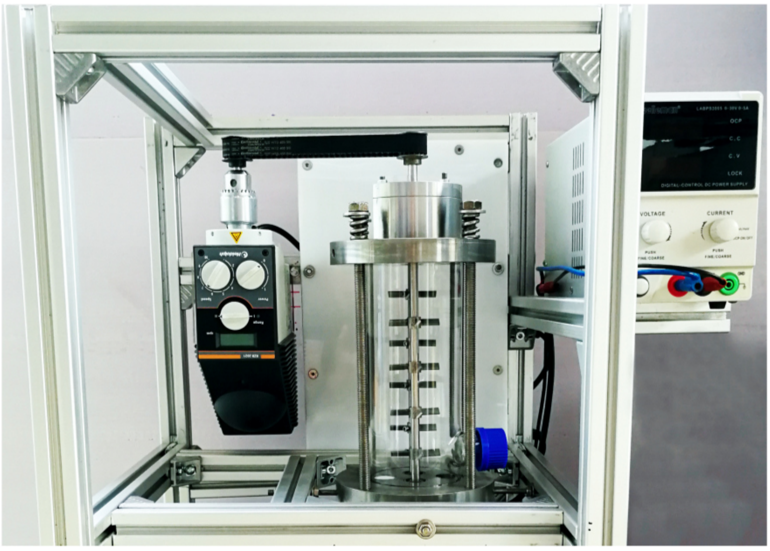
- settling experiment
- ReDrop concept
- coalescence model
- results

PEPs CHEMICAL ENGINEERING

2

LIÈGE université

settling cell



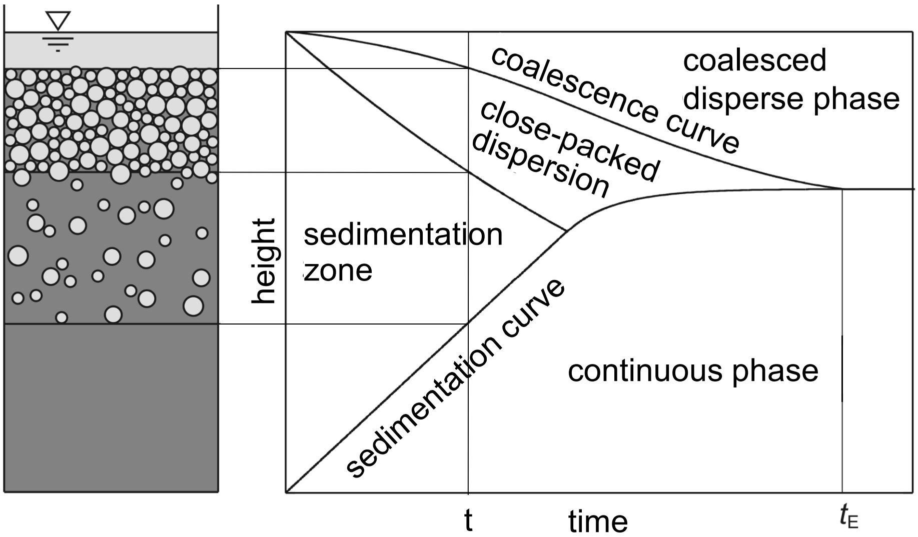
PEPs CHEMICAL ENGINEERING

Leleu, Pfennig (2017). Standardized settling cell to characterize liquid-liquid dispersion. Proceedings of ISEC2017.

3

LIÈGE université

principles of settling



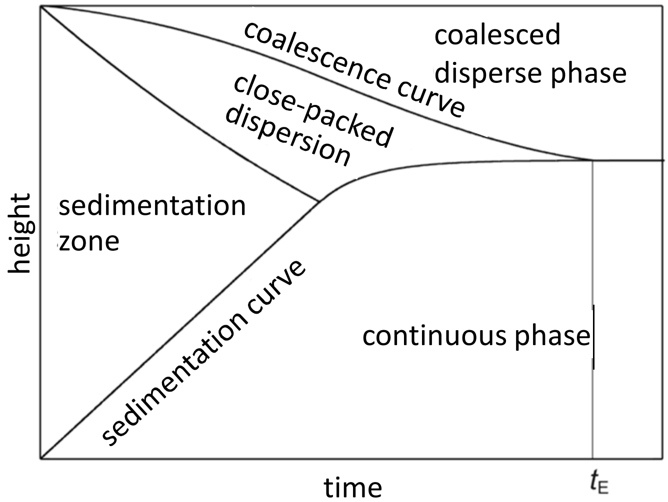
PEPs CHEMICAL ENGINEERING

Henschke, Schlieper, Pfennig (2002). Determination of a coalescence parameter from batch-settling experiments. Chemical Engineering J., 85((2-3)), 369-378.

4

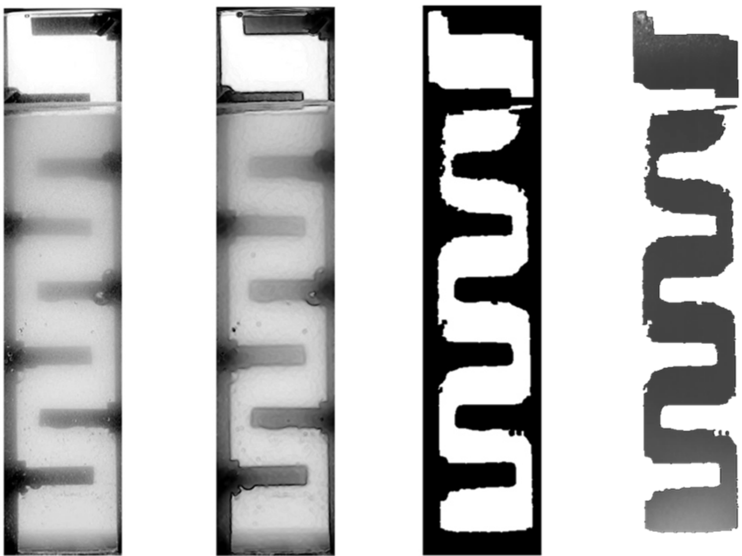
LIÈGE université

principles of settling

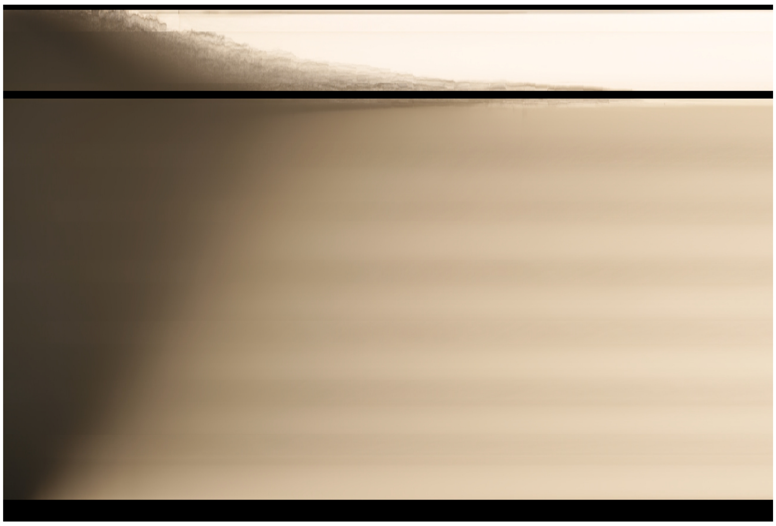


Henschke, Schlieper, Pfennig (2002). Determination of a coalescence parameter from batch-settling experiments. Chemical Engineering J., 85((2-3)), 369-378.

mask of the experiment



experiment evaluation



PEPs CHEMICAL ENGINEERING

LIÈGE université

ReDrop = REpresentative DROPs

- initialization
- data input
- definition of height elements

time loop

for each drop: **drop loop**
- sedimentation velocity
- update position
- coalescence between drops
- coalescence with interface

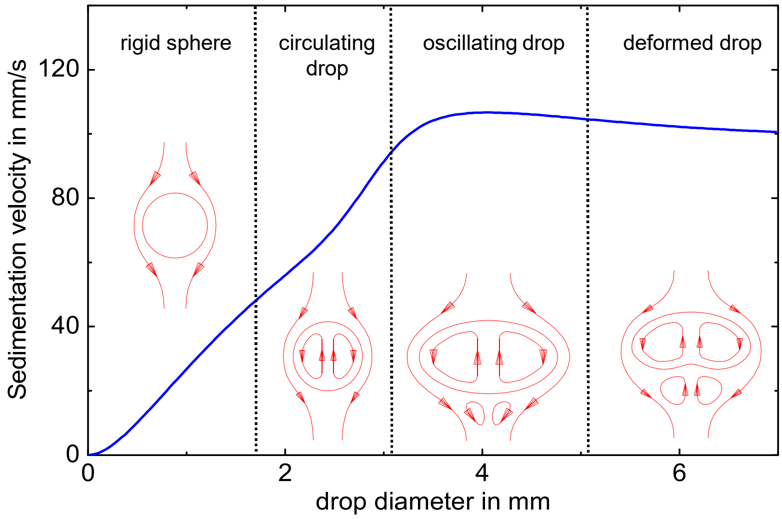
for each height element:
- new hold-up
- new average drop size
- update close-packed zone
- detect settling time

PEPs CHEMICAL ENGINEERING

Leleu, Pfennig, Bruns (2017). Coalescence in Highly Viscous System. Proceedings of ISEC2017.

LIÈGE université

single-drop sedimentation



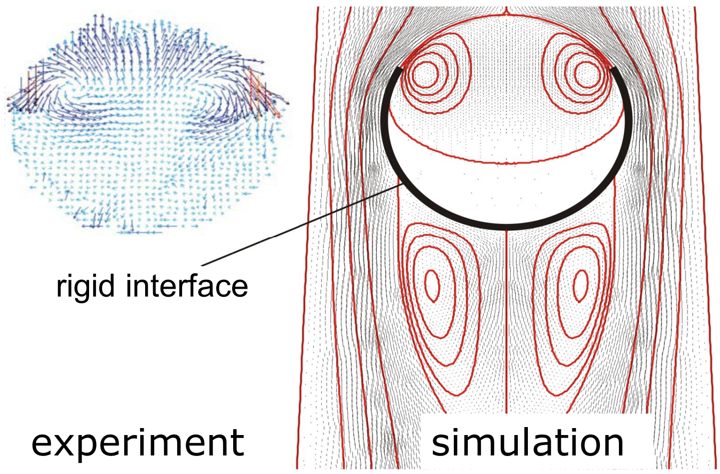
PEPs CHEMICAL ENGINEERING

Kalem, Altunok, Pfennig (2010). Sedimentation behavior of droplets for the reactive extraction of zinc with D2EHPA. AIChE Journal, 56(1), 160-167.
Waheed, Henschke, Pfennig (2004). Simulating sedimentation of liquid drops. International Journal for Numerical Methods in Engineering, 59(14), 1821-1837.

9

LIÈGE université

comparison of simulation and experiment



PEPs CHEMICAL ENGINEERING

Gross-Hardt, Amar, Stapf, Blümich, Pfennig (2006). Flow dynamics measured and simulated inside a single levitated droplet. Industrial and Engineering Chemistry, 45(1), 416-423.

10

LIÈGE université

coalescence model

coalescence frequency

- **collision rate** depends on fluid dynamics
- **bouncing probability** depends on fluid dynamics
- **coalescence probability**
  - **contact time** depends on fluid dynamics
  - **coalescence time** depends on material system

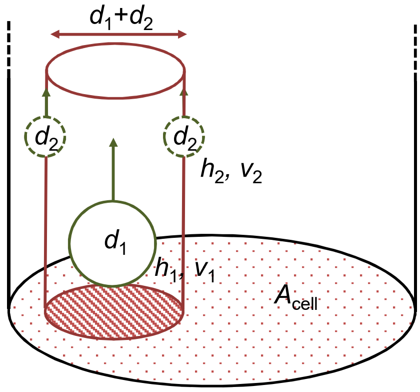
PEPs CHEMICAL ENGINEERING

Kopriwa, Pfennig (2016). Characterization of Coalescence in Extraction Equipment Based on Lab-Scale Experiments. Solvent Extraction & Ion Exchange, 34(7), 622-642.

LIÈGE université

collision frequency

$$r_{collision} = \frac{A_{collision}/A_{cell}}{t_{collision}} = \frac{\pi(d_1+d_2)^2 v_{rel}}{4A_{cell}|h_1-h_2|}$$



PEPs CHEMICAL ENGINEERING

LIÈGE université

free volume after Boublik and Mansoori

contact probability of two drops in polydisperse dispersion

$$g_{ij} = \frac{1}{1-\xi_3} + \frac{6\xi_2 r_i r_j}{(1-\xi_3)^2 (r_i + r_j)} + \frac{8\xi_2{}^2 r_i{}^2 r_j{}^2}{(1-\xi_3)^3 (r_i + r_j)^2}$$

with

$$\xi_m = \frac{\pi N \sum_i x_i (2R_i)^m}{6V}$$

compare: dimensionless density after Carnahan & Starling

$$\eta = \frac{\pi N (2R)^3}{6V} = \varepsilon$$

Kopriwa, Pfennig (2016). Characterization of Coalescence in Extraction Equipment Based on Lab-Scale Experiments. Solvent Extraction & Ion Exchange, 34(7), 622-642.

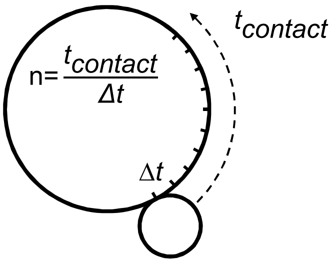
Coulaloglou & Tavlarides

coalescence frequency

- **collision rate** depends on fluid dynamics
- **bouncing probability** depends on fluid dynamics
- **coalescence probability**
  - **contact time** depends on fluid dynamics
  - **coalescence time** depends on material system

$$\omega = h\left(1 - p_{bouncing}\right) \exp\left(-\frac{t_{coalescence}}{t_{contact}}\right)$$

coalescence probability



$$p_{non-coal,n\Delta t} = p_{non-coal,\Delta t}{}^{n}$$

$$p_{non-coal,\Delta t} = \exp\left(-\frac{\Delta t}{t_{coalescence}}\right)$$

$$p_{non-coal,n\Delta t} = \exp\left(-\frac{n\Delta t}{t_{coalescence}}\right)$$

$$p_{non-coal} = exp\left(-\frac{t_{contact}}{t_{coalescence}}\right)$$

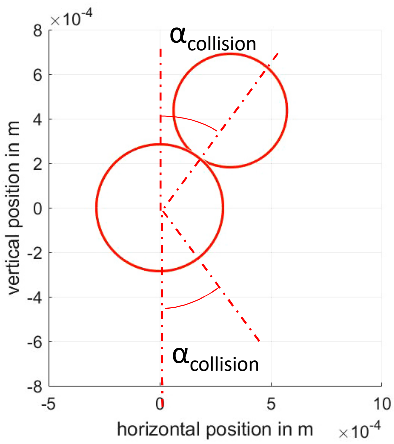
$$p_{coal} = 1 - exp\left(-\frac{t_{contact}}{t_{coalescence}}\right)$$

PEPs CHEMICAL ENGINEERING

15

LIÈGE université

coalescence model: contact time



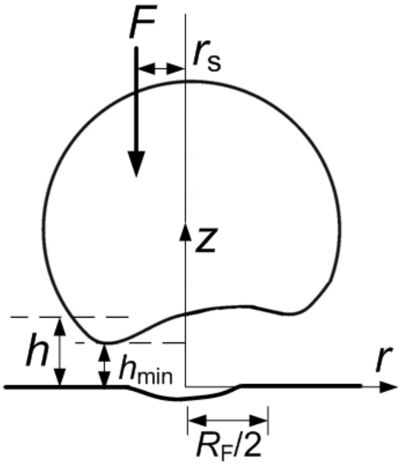
- assumptions:
  - drops follow contour during the sedimentation
  - detachment angle = opposite of the collision angle

PEPs CHEMICAL ENGINEERING

16

LIÈGE université

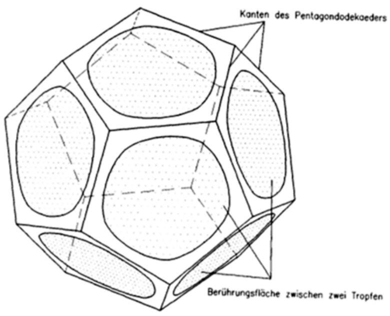
coalescence time, asymmetric dimple

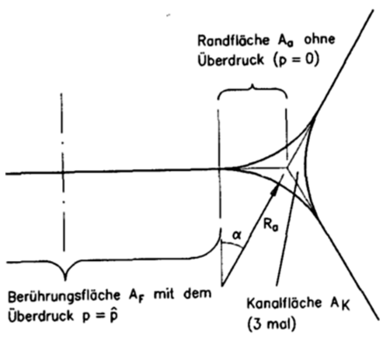


$$t_{coalescence} = \frac{3\pi^{1.5}\mu R_{eq}^2}{4 r_s^* \sqrt{\sigma F_{driving} h_{min}}}$$

Henschke, Schlieper, Pfennig (2002). Determination of a coalescence parameter from batch-settling experiments. Chemical Engineering J., 85((2-3)), 369-378.
Pfennig, Schwerin (1995). Analysis of the Electrostatic Potential Difference in Aqueous Polymer 2-Phase Systems. Fluid Phase Equilibria, 108((1-2)), 305-315.

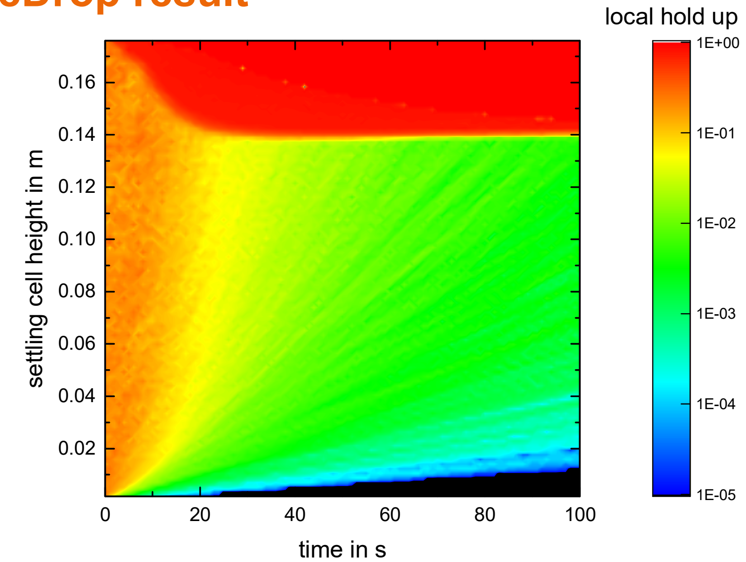
dodecahedron deformation after Henschke



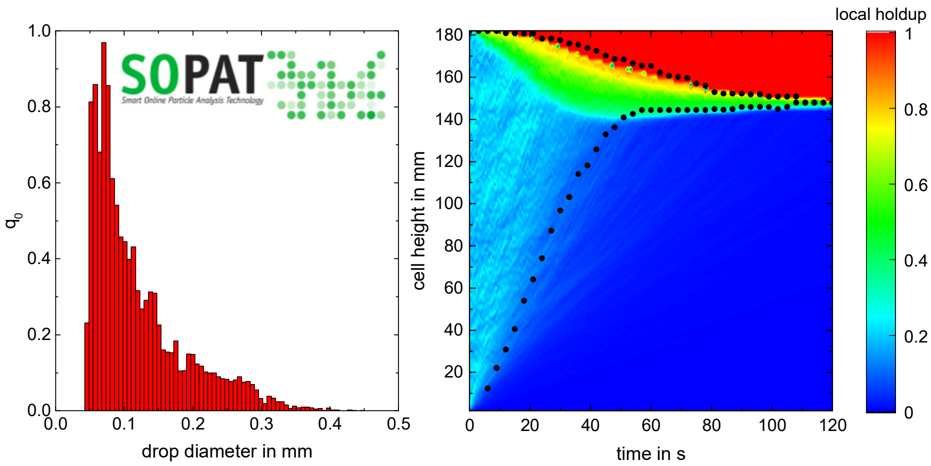


Henschke, Schlieper, Pfennig (2002). Determination of a coalescence parameter from batch-settling experiments. Chemical Engineering J., 85((2-3)), 369-378.

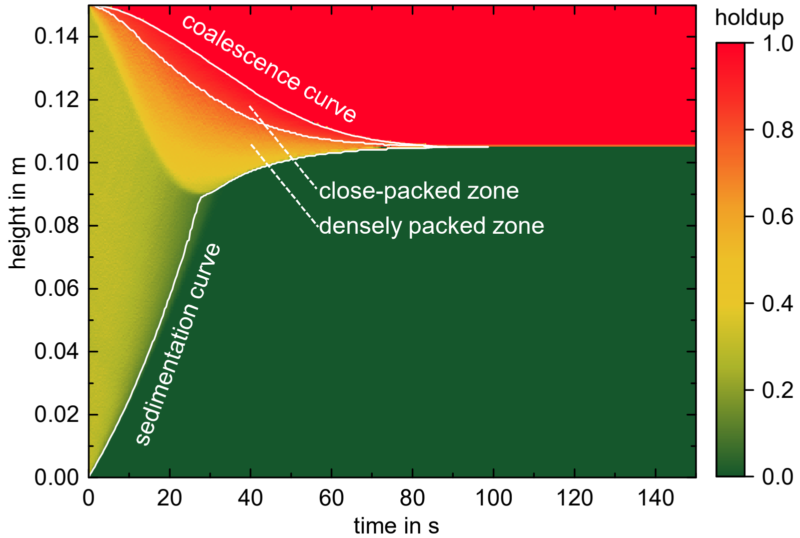
ReDrop result



status of the model validation



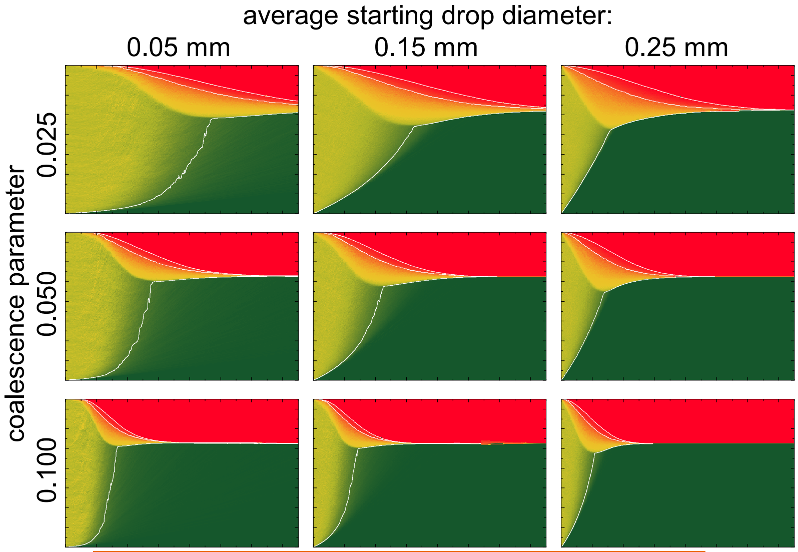
ReDrop result



PEPs CHEMICAL ENGINEERING

LIÈGE université

lag time & system-typical effective diameter



PEPs CHEMICAL ENGINEERING

LIÈGE université

conclusions

- drop-based model $\rightarrow$ detailed results
- high-holdup flow $\rightarrow$ densely-packed zone
- sedimentation coalescence
  $\rightarrow$ lag time
  $\rightarrow$ system-typical effective diameter
- consistent modelling of coalescence

PEPs CHEMICAL ENGINEERING

23

LIÈGE université

8th International Berlin Workshop (IBW 8) on
Transport Phenomena with Moving Boundaries
25th - 26th October 2018, Berlin, Germany

Drop-based modelling of coalescence in batch settlers including polydispersity

ERICAA

Supported by:
Federal Ministry for Economic Affairs and Energy
on the basis of a decision by the German Bundestag

David Leleu, Andreas Pfennig
andreas.pfennig@uliege.be
Products, Environment, and Processes (PEPs)
Department of Chemical Engineering
Université de Liège
www.chemeng.uliege.be/Pfennig

PEPs CHEMICAL ENGINEERING

LIÈGE université 200