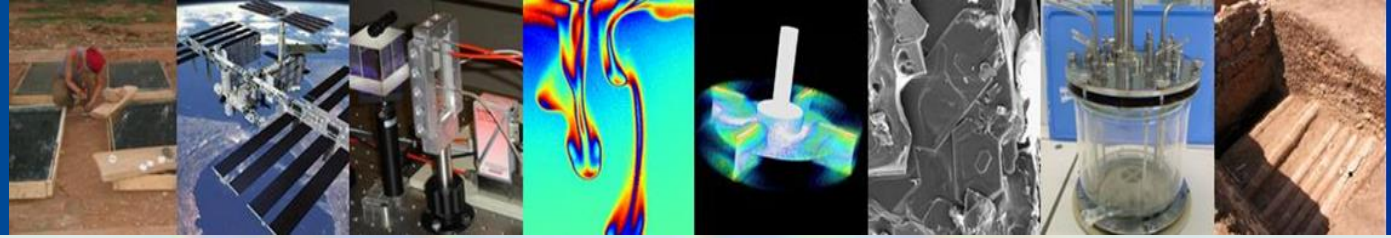
ULB



Transfers, Interfaces & Processes

Simulation of gravitational instability during CO_2 absorption in a $NaHCO_3/Na_2CO_3$ solution

C. Wylock, A. Rednikov, B. Haut and P. Colinet

COMSOL CONFERENCE ROTTERDAM 2013

October 23 - 25, 2013

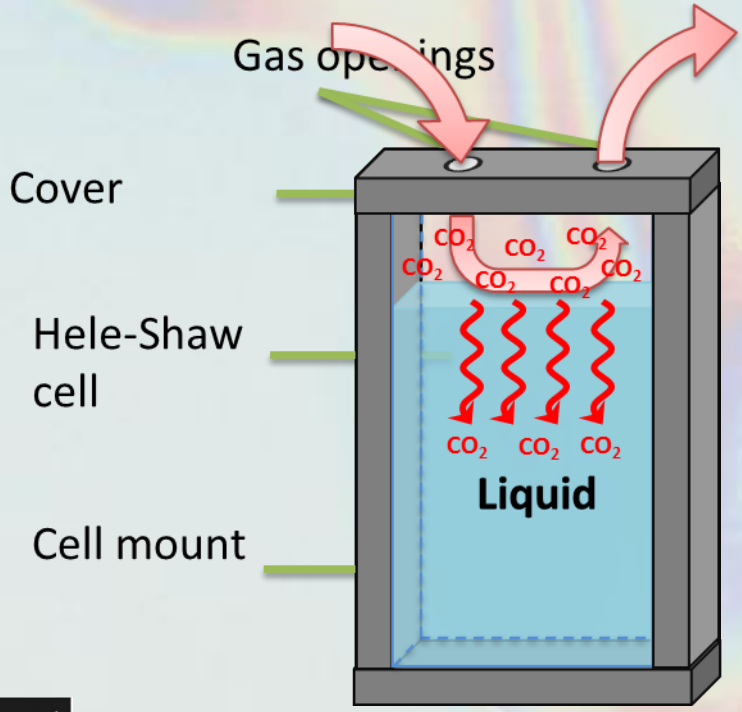
WTC Rotterdam

ECOLE POLYTECHNIQUE DE BRUXELLES

fnrs FREEDOM TO RESEARCH

ULB Framework

- **Study of gas-liquid CO_2 absorption into reactive solution in a Hele-Shaw cell for**
  - environnemental technologies (e.g. CO_2 scrubbing)
  - process intensification involving CO_2 (e.g. Solvay process)



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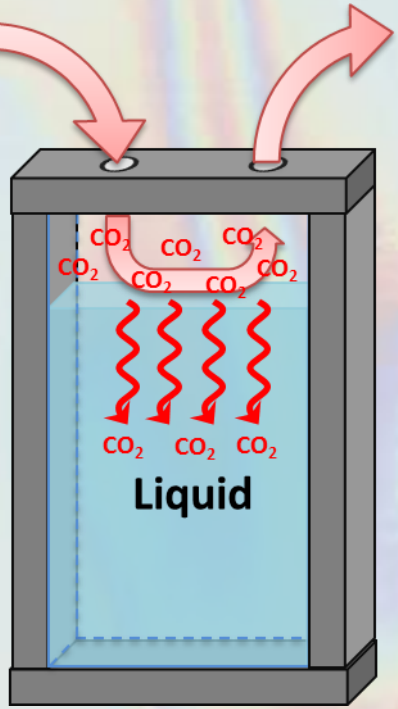
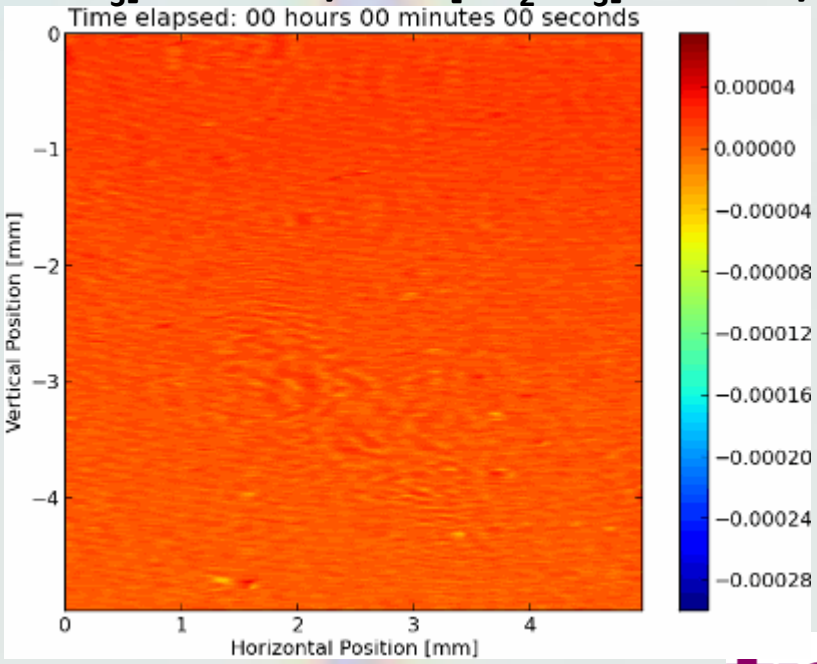


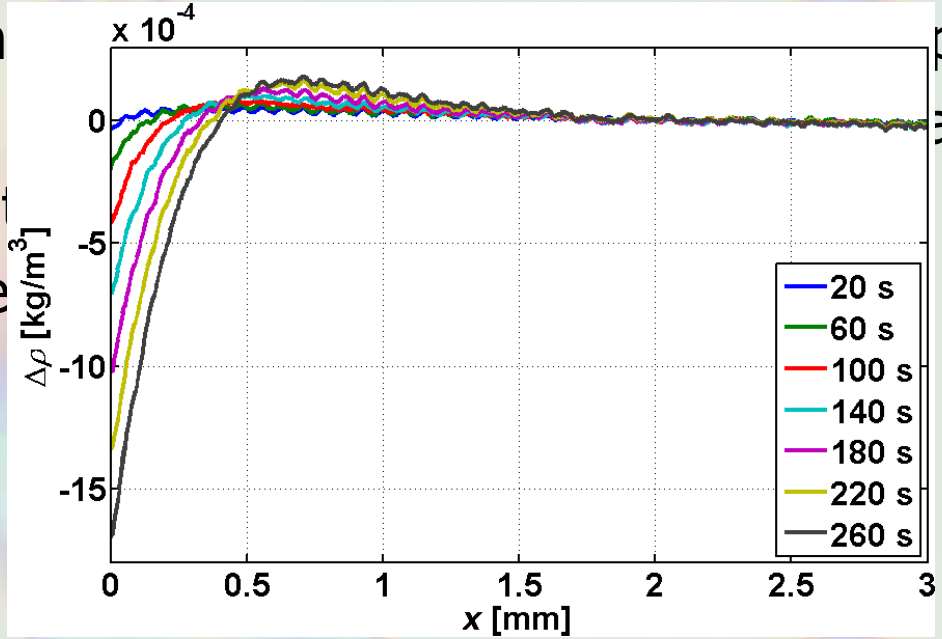
$[NaHCO_3]$=790 mol/m³ – $[Na_2CO_3]$=625mol/m³



FREEDOM TO RESEARCH

ULB Framework

- **Instability behavior due to the particular shape of density variation profile before instability onset generated by the chemical reactions [1]**
- **DNS of transport equations in order to:**
  - Betterly un phenomena
  - Assess the absorption rate
  - Identify cri
  - Investigate



[1] MGST 20, p.171-175

Mathematical modelling

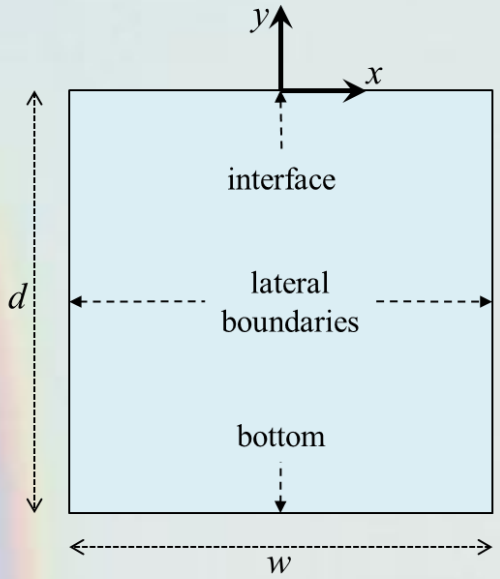
- **Assumptions**
  - Only liquid phase considered
  - Liquid thickness << depth & width → 2-D domain
  - Interfacial reaction A + B → C (A from gas, B and C in liquid)
  - Density variation are related only to :
    - Diffusivity ratio: $D^* = \frac{D_C}{D_B}$
    - Contribution to density ratio: $\varrho^* = \frac{\frac{\partial \rho}{\partial [C]}}{\frac{\partial \rho}{\partial [B]}}$

Mathematical modelling

- **Computational domain**
- **Normalized transport equations**
  - Concentrations :

$$\frac{\partial [B]}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}[B] = \boldsymbol{\nabla}^2[B]$$

$$\frac{\partial [C]}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla}[C] = D^* \boldsymbol{\nabla}^2[C]$$



  - Momentum (Navier-Stokes-Darcy[2]) :

$$\mathrm{Sc}^{-1}\left(\frac{\partial \boldsymbol{u}}{\partial t} + \frac{6}{5}\boldsymbol{u} \cdot \boldsymbol{\nabla}\,\boldsymbol{u}\right) + \mathrm{Br}\,\boldsymbol{u} = -\boldsymbol{\nabla} p + \boldsymbol{\nabla}^2 \boldsymbol{u} - \mathrm{Ra}\,\Delta\rho\,\boldsymbol{e}_y$$

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

$$\Delta\rho = \sigma\big(([B] - 1) + \varrho^*([C] - C_0)\big)$$

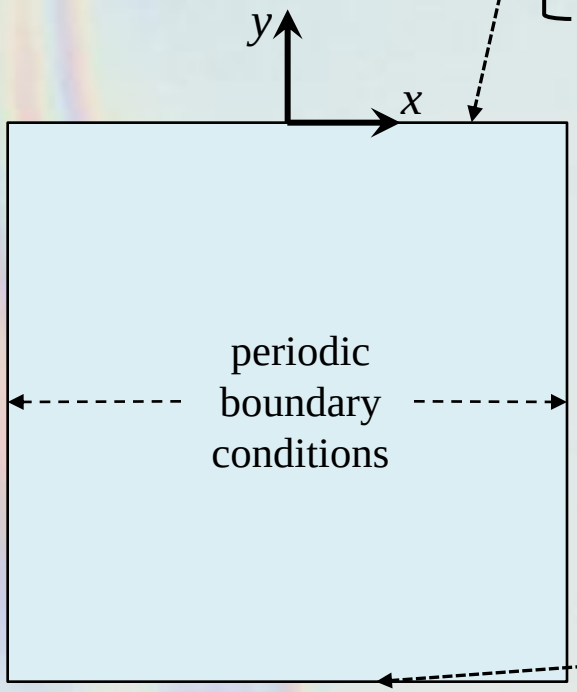
[2] PoF 14(2), p.902-905

Mathematical modelling

- **Boundary conditions**

$$[B] = 0 \; ; D^* \frac{\partial [C]}{\partial y} = -\frac{\partial [B]}{\partial y}$$

$$v = 0 \; ; \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0$$

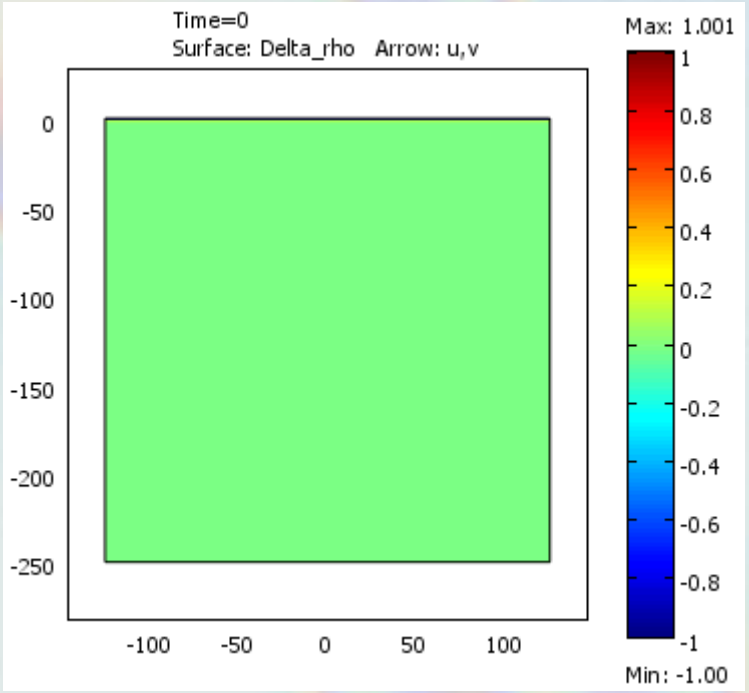


$$\frac{\partial [B]}{\partial y} = 0 \; ; \; \frac{\partial [C]}{\partial y} = 0$$

$$\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} = 0 \; ; \; -p + \frac{\partial v}{\partial y} = 0$$

Results and discussion

- **Analysis of time evolution of $\Delta\rho$ field**

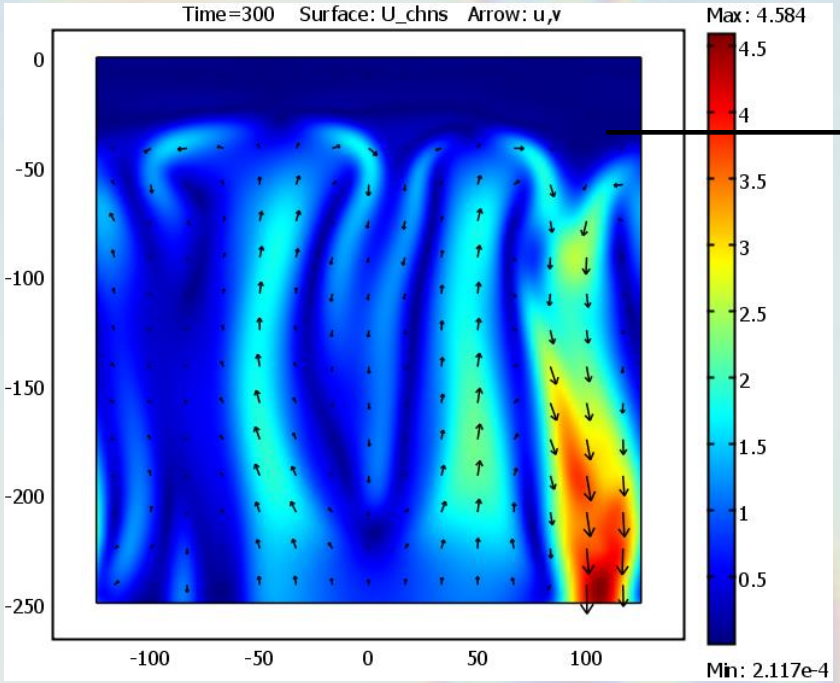


- Start with homogeneous penetration stage
- Plumes appear at a small from interface while liquid close to interface seems to remain homogeneous
- Plumes sinking at the onset, slowing down before a new « burst »

→ Reproduce rather well the experimentally observed behavior !

Results and discussion

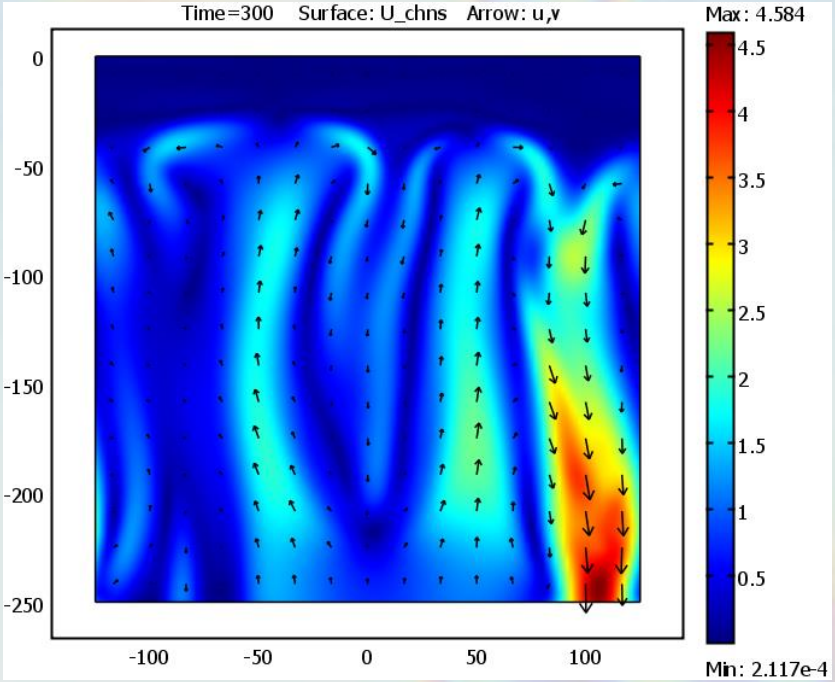
- **Analysis of velocity field and absorption rate**

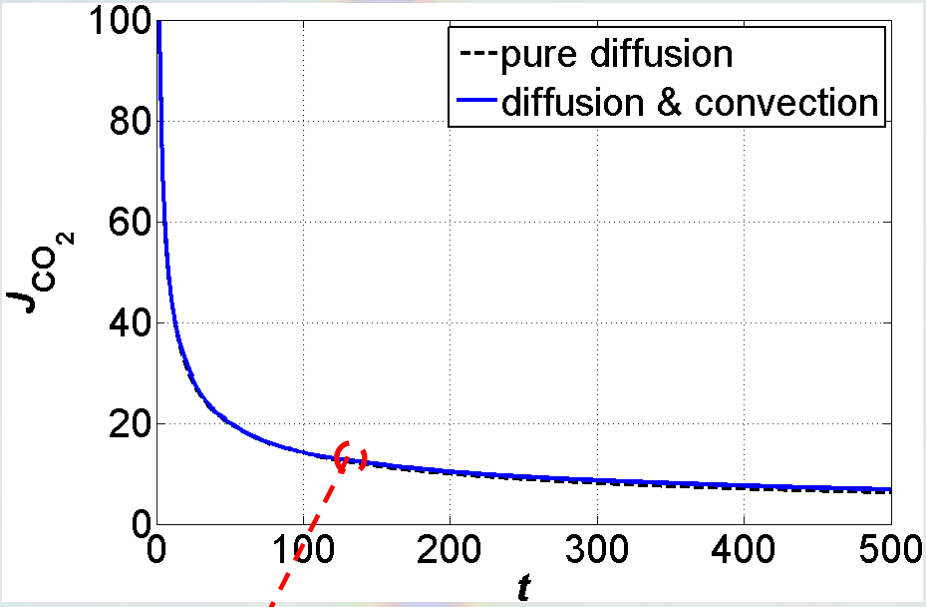


Close to interface, liquid remains quiescent
→ effect on mass absorption rate ?

Results and discussion

- **Analysis of velocity field and absorption rate**





No significant enhancement compared to pure diffusion after instability onset

→ absorbed mass has still to diffuse through a quiescent liquid layer

Conclusion

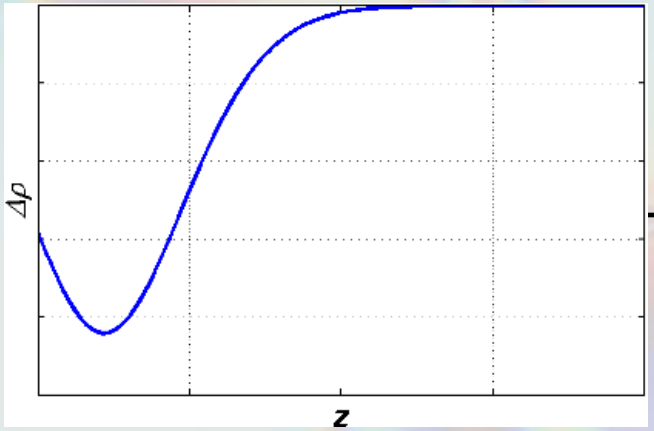
- **DNS results similar to experimental observation of CO_2 absorption in $NaHCO_3/Na_2CO_3$ solution**

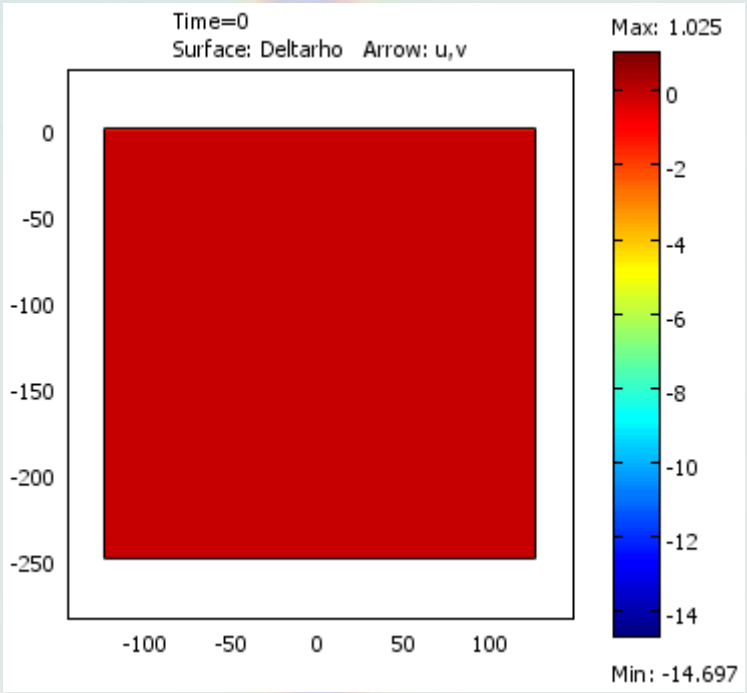
→ **Validate the model and the numerical procedure**

- **Better understanding of the phenomena coupling and their influence**
- **Analysis of important variables**
  - Stratified instability with quiescent and non-quiescent zones
  - No significant effect of instability on mass absorption rate

ULB Perspective

- **Identify new experimental system leading other unusual instability behaviors**





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Thanks for your kind attention

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