Hydrodynamics And Mass Transfer In Taylor Flow

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Overview

I. Modelling Strategy

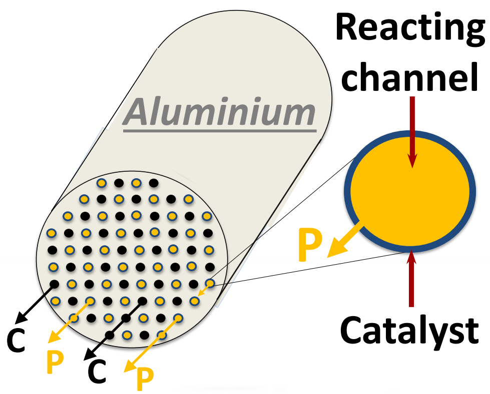
II. Liquid-phase hydrodynamics

III. Gas-liquid mass transfer

IV. Conclusions and Recommendations

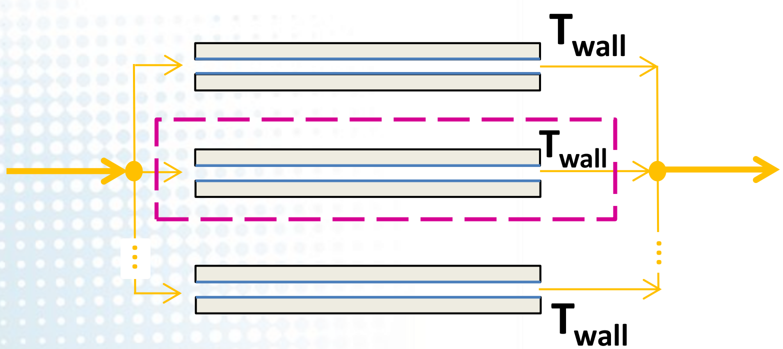
Modelling strategy

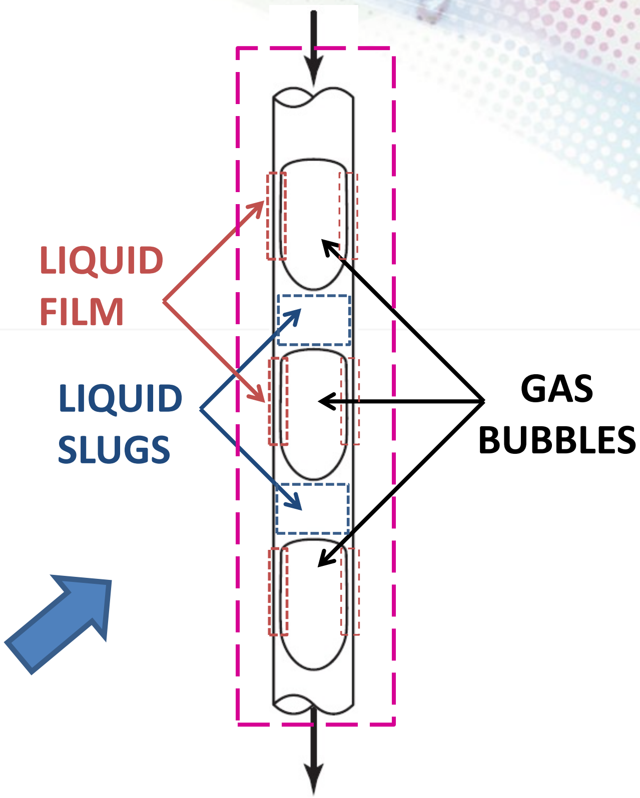
Monolith reactor



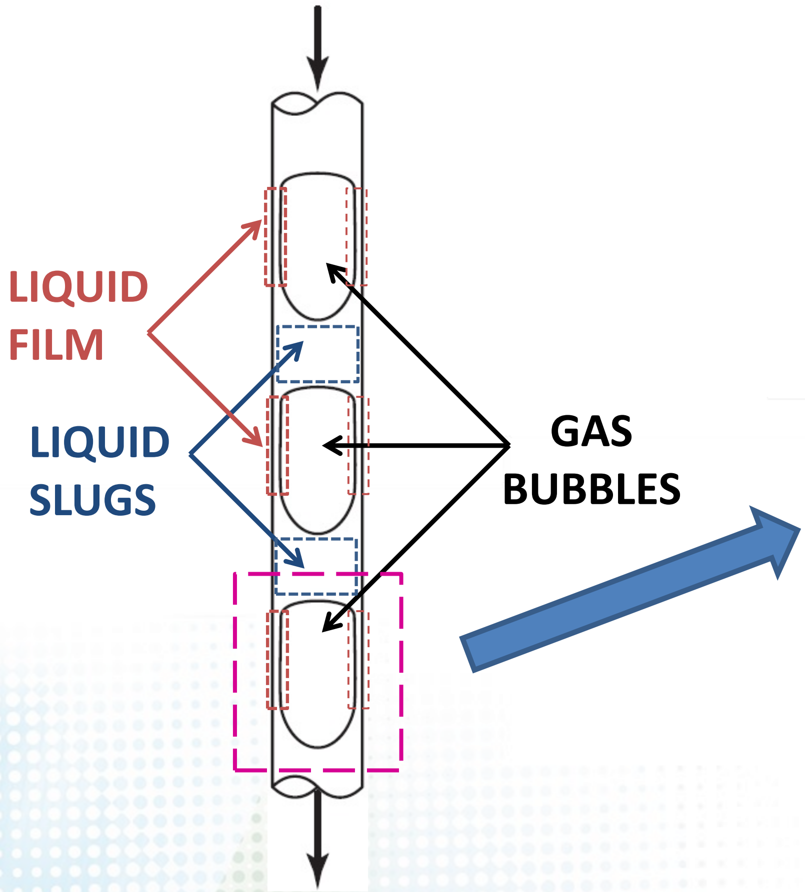
P: Product
C: Coolant

Single-channel approach

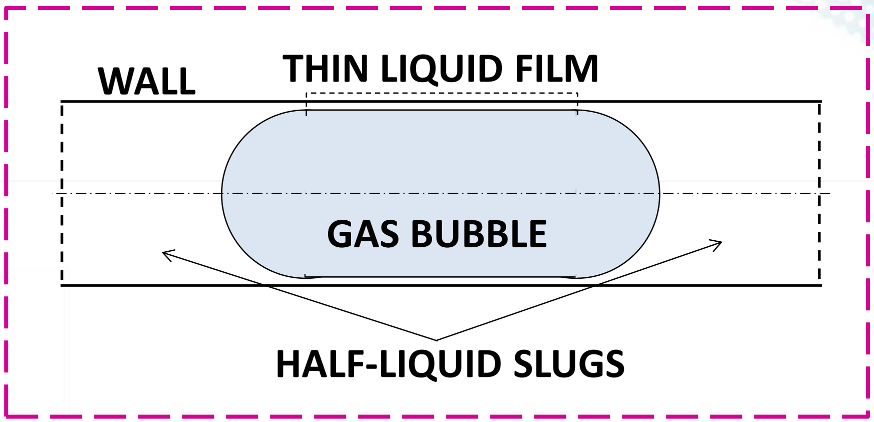




Modelling strategy



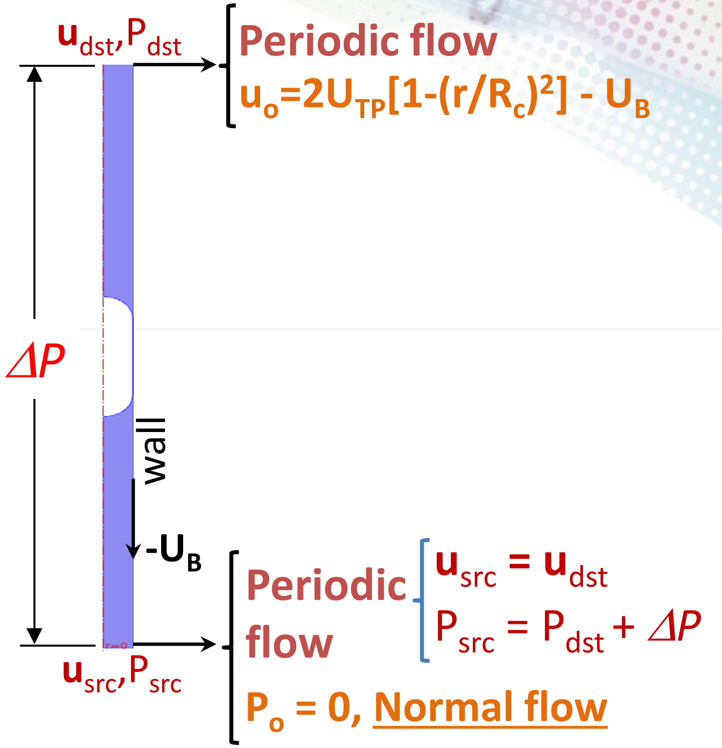
Fully-developed Taylor flow



Unit Cell approach (UC):

- Bubble frame of reference.
- Bubble fixed shape.
- P & **u** fields as numerical "platform" to mass transfer.

Liquid-phase hydrodynamics



Simulation Strategies

1. ***Periodic UC***: Periodic B.C. in the vert. direction
   → $u_{source} = u_{destination}$, $P_{source} = P_{destination} + \Delta P$
2. ***"Open" UC:*** Parabolic velocity profile (inlet);
   P = 0, normal flow (outlet)
   → ΔP evaluation & comparison

Governing equations

Mass conservation:

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

Momentum conservation (upward flow):

$$\rho_L(\boldsymbol{u}_L \cdot \nabla)\boldsymbol{u}_L = \nabla \cdot [-p\boldsymbol{I} + \mu(\nabla \boldsymbol{u}_L + (\nabla \boldsymbol{u}_L)^T)] + \boldsymbol{F}$$

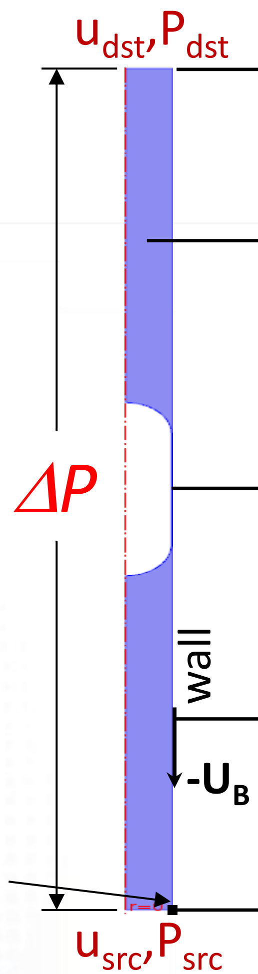
Liquid-phase hydrodynamics

Periodic Unit Cell strategy → $\vec{u}_{src} = \vec{u}_{dst}$, $P_{src} - P_{dst} = \Delta P$?

Remarks:

- Van Baten & Krishna study case[1]
- Upward concurrent flow
- Bubble frame of reference
- Air-water system

[1]van Baten, J.M., Krishna, R., *Chem Eng Sci*. 2004, 59, 2535-2545



Periodic flow

Laminar flow
- Liquid properties: ρ_L, μ_L
- $\mathbf{F}_{vol}$: $-\rho_L * \boldsymbol{g}$

G-L interface:
Slip / No slip

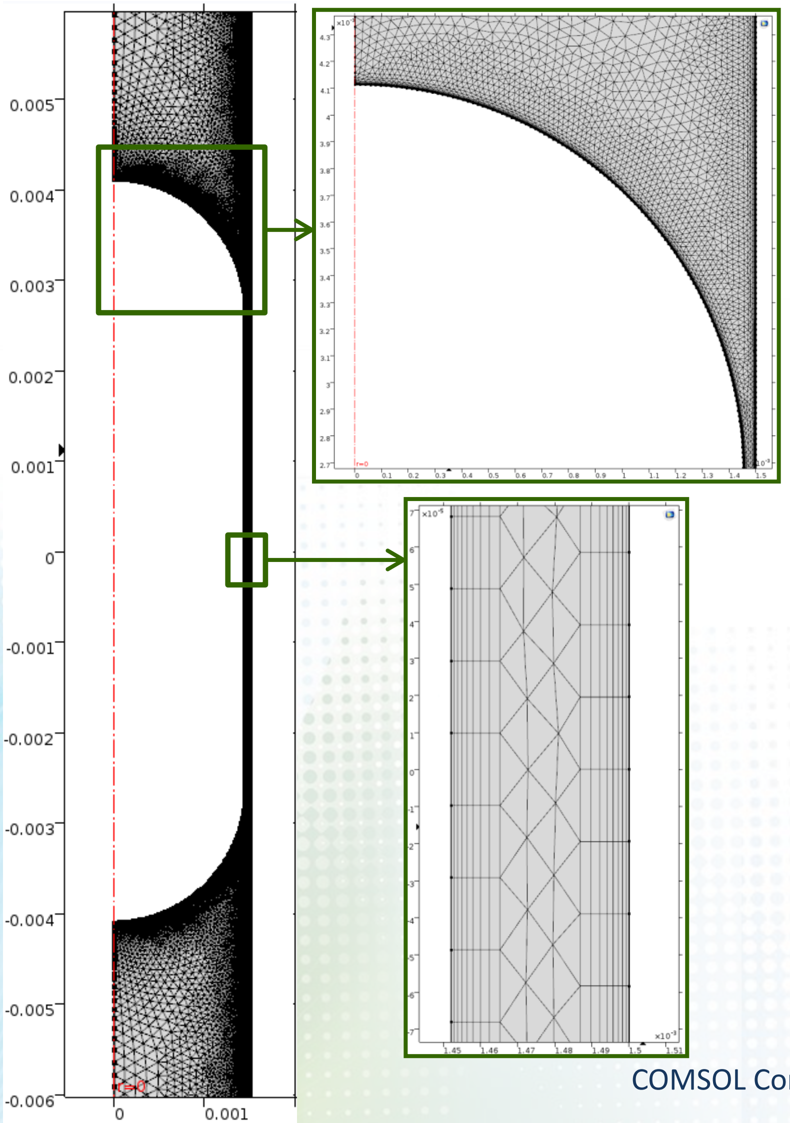
Moving wall = $-U_B$

Pressure ref.: P_o = 0 bar

Periodic flow
- $\mathbf{u}_{src} = \mathbf{u}_{dst}$
- $P_{src} = P_{dst} + \Delta P$

Liquid-phase hydrodynamics

Mesh 2 with focus on refined zones

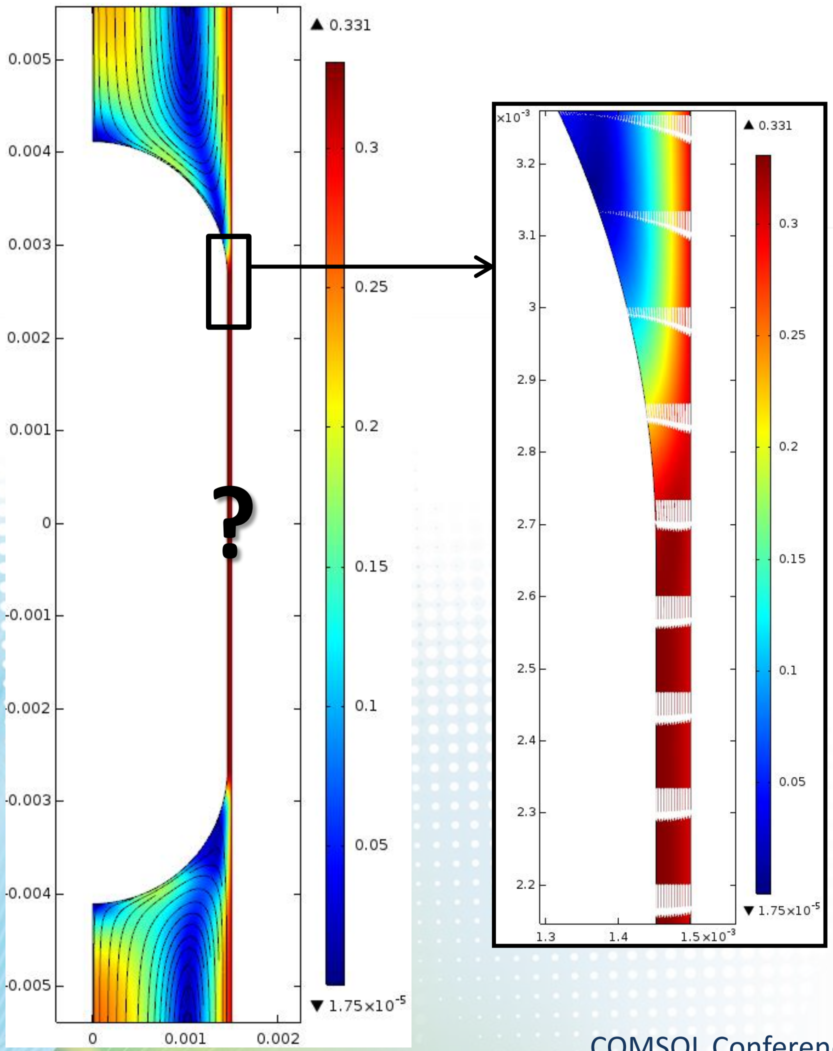


Mesh details for the sensitivity study

	Total mesh element	Smallest element size (µm)	Biggest element size (µm)	N. of elem. in liq. film	ΔP_{OpenUC} (Pa)
1	33347	3	155	17	283
2	77318	~0,8	155	19	324
3	151616	~0,2	87	22	331
4	226798	~0,2	67	22	325

Liquid-phase hydrodynamics

Results: converged velocity fields in *periodic UC*, ΔP_{calc}



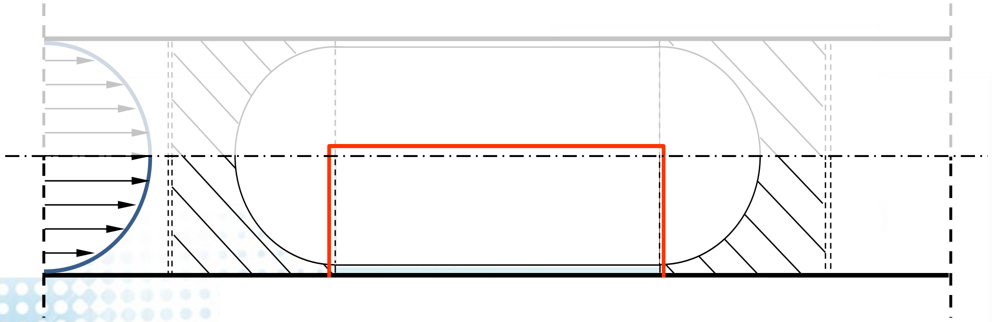
Remarks:

- ✓ Parabolic profile within the slug.
- ✓ U_{max} changes by ~15% between $\Delta P = 0$ and ΔP calculated in *open UC* (ΔP_{OpenUC}).
- ✓ Fully-developed flow on the liquid film is rapidly observed.

Liquid-phase hydrodynamics

Comparison of the B.C. at the interface between simulations and Abiev's[1] model

Analysis of a *"fully-developed film-bubble flow"*:



Gas phase:

$$0 = -\frac{dp}{dz} + \rho_G g + \mu_G \left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dV_{zG}}{dr}\right)\right]$$

Liquid phase:

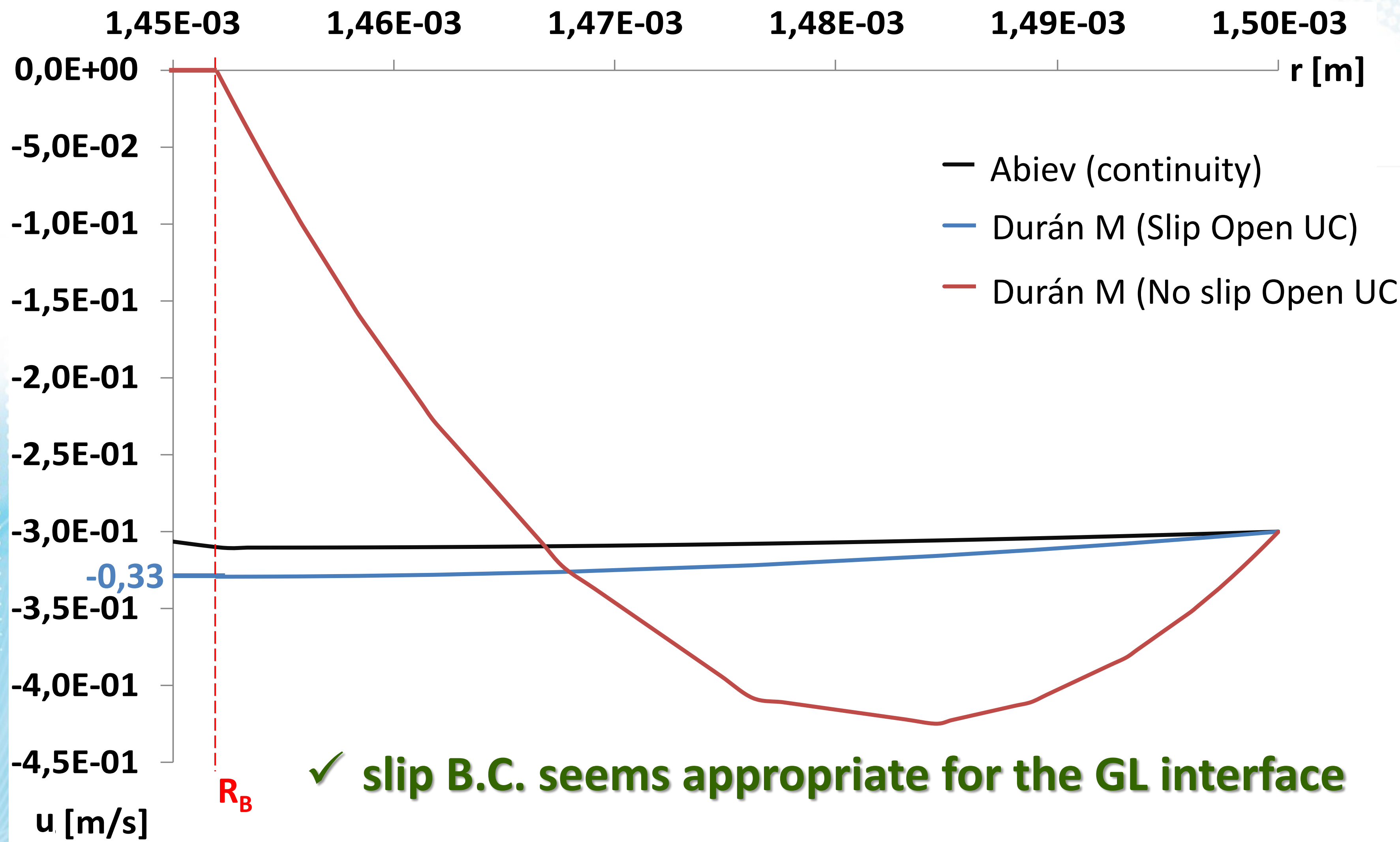
$$0 = -\frac{dp}{dz} + \rho_L g + \mu_L \left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dV_{zL}}{dr}\right)\right]$$

$$\frac{dp_G}{dz} = \frac{dp_L}{dz} = \frac{dp}{dz}$$

[1]Abiev, R.Sh., Theor Found Chem Eng. 2008, 42, 1105-117

Liquid-phase hydrodynamics

Comparison of the B.C. at the interface between simulations and Abiev's[1] model



✓ slip B.C. seems appropriate for the GL interface

Mass transfer

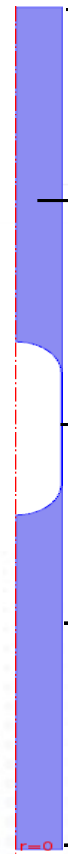
Stationary mass transfer with reaction at the wall

Aim:

- Stationary: Transfer ↔ Rxn
- $k_L a$ evaluation & comparison

Remarks:

- Bubble: *mass source*
- Reactive wall: *mass sink*
- Bubble frame of reference
- Air-water system



Periodicity

Convection & diffusion

$$\nabla.(-D_i \nabla c_i) + \mathbf{u}.\nabla c_i = R_i$$
$$\mathbf{N}_i = -D_i \nabla c_i + \mathbf{u} c_i$$
Periodic velocity field **u**
D_i : 10^{-9} [m^2/s]

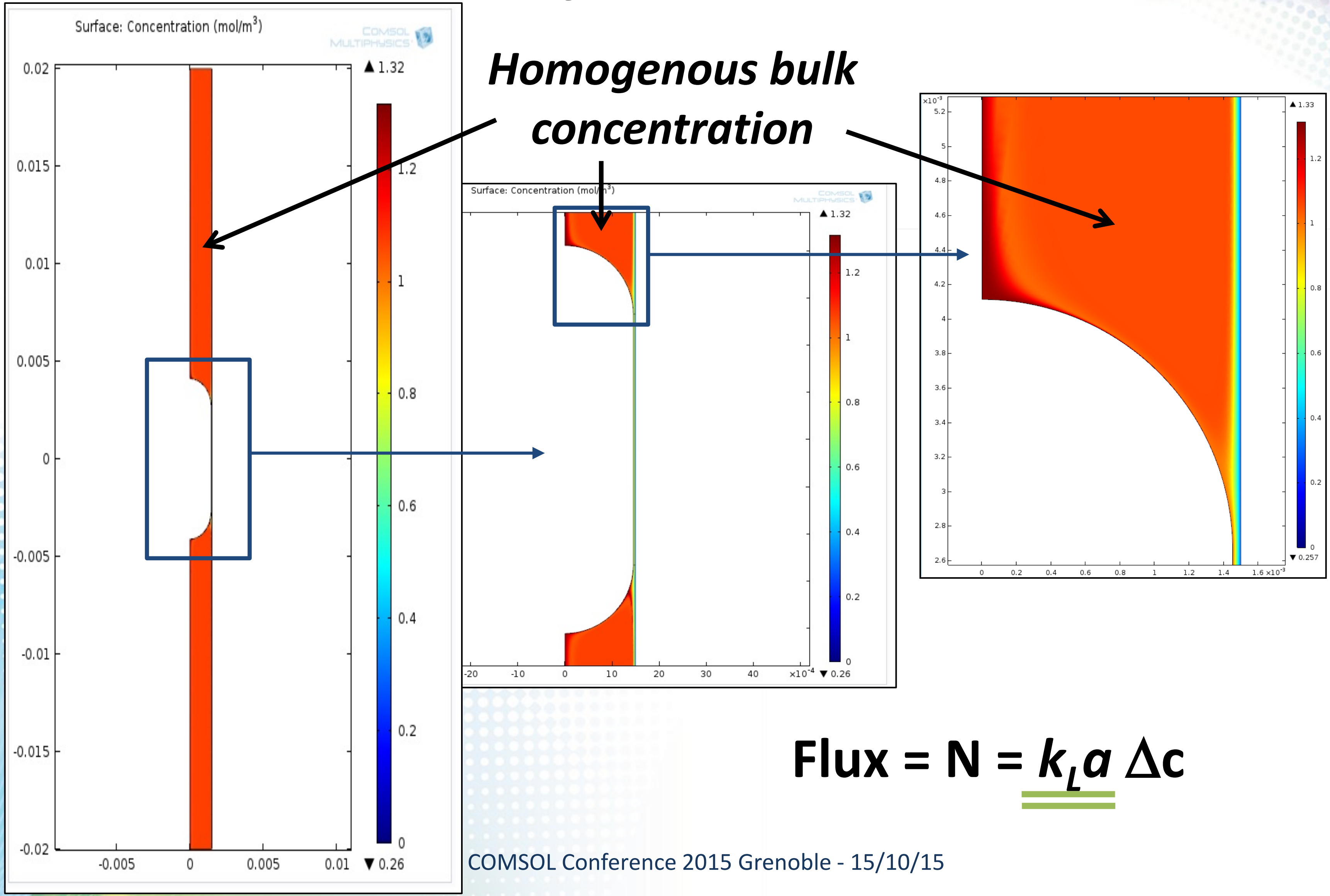
G-L Interface:
$c^* = 1{,}3$ mol/m^3

Flux: $- \mathbf{n} . \mathbf{N}_i = K_c * c$ [mol/m^2/s]

Periodicity
$$c_{i,\text{in}} = c_{i,\text{out}}$$
$$-\mathbf{n}_{\text{in}} . \mathbf{N}_{i,\text{in}} = -\mathbf{n}_{\text{out}} . \mathbf{N}_{i,\text{out}}$$

Mass transfer

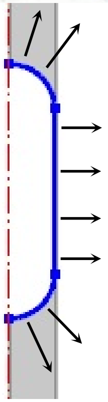
Stationary concentration field



$$\text{Flux} = N = \underline{\underline{k_L a}}\,\Delta c$$

Mass transfer

Methodology for $k_L a$ evaluation



Gas molar flow rate from bubble:

N = Surface integration(**chds.bndFlux_c**) [mol/s] (1)

N = I/S_{bubble} [mol/m²/s]

Overall average concentration $\langle C_{overall} \rangle$:

$\langle C_{overall} \rangle$ = Volume integration(**c**)/V_L [mol/m³] (2)

$$k_L a = \frac{N}{(C^* - \langle C_{overall} \rangle)} * \frac{bubble\ surface\ area}{UC\ volume} = 0.078 \left[\frac{m_L^3}{m_{UC}^3 * s}\right] \quad (3)$$

Conclusions & Recommendations

Conclusions

- ✓ Methodology for a relevant ΔP choice has been developed.
- ✓ Periodic UC → ΔP influence has been shown.
- ✓ Slip B.C. seems appropriate after comparison.
- ✓ $k_L a$ has been computed in a reaction study case.

Future work

- ✓ Complex kinetic equation → heterogeneous catalyst on the wall
- ✓ Add heat transport
- ✓ Build a overall monolith reactor model

Acknowledgements

THANK YOU!

Questions