



Bubble Dissolution in Taylor-Couette flow

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Outline

- 1. Motivation
- 2. Description of the problem
- 3. Numerical Framework
- 4. Taylor-Couette flow: single-phase validation
- 5. Mass transfer in Taylor-Couette flow
- 6. Conclusions





Motivation

Mass transfer of soluble species

• Mass transfer of soluble species occurs in many natural and industrial systems.





• Air-Sea gas transfer



- Chemical reactors
- Green production of hydrogen

- Complex physics (multi-phase flow, interfacial discontinuity, reactive species).
- Design models rely on simplified correlation formulae.





Problem description

Soluble species in bubbly flows

- Disperse bubbly flow
- Soluble species in the liquid







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Problem description

Soluble species in bubbly flows

Disperse bubbly flow







Problem description

Soluble species in bubbly flows

Disperse bubbly flow







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Numerical framework

Direct Numerical Simulations of two-phase flows



- Incompressible DNS + geometric VOF
- Phase-change model

$$\nabla \cdot \boldsymbol{u} = \dot{m} \left(\frac{1}{\rho_d} - \frac{1}{\rho_c} \right) \delta_{\Sigma}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot (\boldsymbol{u} \otimes \boldsymbol{u}) = \frac{1}{\rho} [-\nabla p + \nabla \cdot (2\mu \boldsymbol{D})] + \frac{\sigma k \boldsymbol{n}_{\Sigma}}{\rho} \delta_{\Sigma}$$
$$\frac{\partial f}{\partial t} + \nabla \cdot (\boldsymbol{u} f) = -\frac{\dot{m}}{\rho_c} \delta_{\Sigma}$$







Transport of species Two-scalar approach

• Two scalar equations for each species

$$\frac{\phi_c^{n+1} - \phi_c^n}{\Delta t} V + \oint_{\partial V_c \setminus \Sigma} c_c \boldsymbol{u}_c \cdot \boldsymbol{n} \, ds - \oint_{\partial V_c \setminus \Sigma} D_c \nabla c_c \cdot \boldsymbol{n} \, ds = -\oint_{\Sigma} \frac{\dot{m}}{M} \, ds$$

$$\frac{\phi_d^{n+1} - \phi_d^n}{\Delta t} V + \oint_{\partial V_d \setminus \Sigma} c_d \boldsymbol{u_d} \cdot \boldsymbol{n} \, ds - \oint_{\partial V_d \setminus \Sigma} D_d \nabla c_d \cdot \boldsymbol{n} \, ds = + \oint_{\Sigma} \frac{\dot{m}}{M} \, ds$$



Transport of species Two-scalar approach

• Two scalar equations for each species

- Species confined within the respective phase during advection/diffusion
- Advection: tracers associated to VOF field
- Diffusion coefficient weighted by the face fraction field [*]

* Magdelaine-Guillot de Suduiraut, Q., 2019. Hydrodynamique des films liquides hétérogènes. Thesis. Sorbonne Université.



Mass transfer rate

A geometric scheme

Diffusion-driven mass transfer (Fick's law)

$$-\frac{\partial c_c}{\partial n_{\Sigma}} = f_P \frac{c_c(P_1) - c_c(P)}{PP_1} + (1 - f_P) \frac{c_c(P_2) - c_c(P)}{PP_2} [*]$$

•
$$c_c(P) = \frac{c_d(P)}{H_e}$$
 (Henry's law)



* Bothe, D., Fleckenstein, S., 2013. A volume-of-fluid-based method for mass transfer processes at fluid particles. Chem. Eng. Sci. 101, 283–302.



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Coupling with a geometric VOF method Incompatibility issue

- Geometric VOF method [*] •
- Kinematic constraint:

$$\frac{\Delta t}{\Delta} H_{(i,j)} \nabla_{\Delta} \cdot \boldsymbol{u} = 0$$
$$H_{(i,j)} = \begin{cases} 1 & \text{if } f > 0.5\\ 0 & \text{Otherwise} \end{cases}$$

^{*} Weymouth, G.D., Yue, D.K.P., 2010. Conservative volume-of-fluid method for free-surface simulations on cartesian-grids. J. Comput. Phys. 229, 2853–2865.





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Always true for incompressible flows without mass transfer

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Bubble with constant mass transfer rate

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Coupling with a geometric VOF method Velocity extension

• Always true in pure gas cells $(H_{(i,j)} = 0)$

 $\frac{\Delta t}{\Lambda} H_{(i,j)} \nabla_{\Delta} \cdot \boldsymbol{u} = 0$





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Mass transfer redistribution [*,**]



^{*} Gennari, G., Jefferson-Loveday, R., Pickering, S. J., 2022. A phase-change model for diffusion-driven mass transfer problems in incompressible two-phase flows. Chem. Eng. Sci. 259 117791.

^{**} Boyd, B., Ling, Y., 2023. A consistent volume-of-fluid approach for direct numerical simulation of the aerodynamic breakup of a vaporizing drop. Computers & Fluids 254 105807.





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Mass transfer redistribution [*,**]



$$avg_{(i,j)} =$$
pure gas cells $\Big|_{3\times 3}$

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Coupling with a geometric VOF method Velocity extension Ω_{c}

• Always true in pure gas cells $(H_{(i,i)} = 0)$

 $\frac{\Delta t}{\Lambda} H_{(i,j)} \nabla_{\Delta} \cdot \boldsymbol{u} = 0$

Mass transfer redistribution [*,**]



$$avg_{(i,j)} =$$
pure gas cells $\Big|_{3\times 3}$

 $\dot{m}'_{(i,j)} = \sum_{2\times 2} \frac{m_{(l,k)}}{avg_{(l,k)}} A_{\Sigma(l,k)}$ j Ω_d 2

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Validation

Velocity extension





Validation

0

-300





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Validation

Rising bubble at different Péclet numbers



* Takemura, F., Yabe, A., 1998. Gas dissolution process of spherical rising gas bubbles. Chem. Eng. Sci. 53, 2691–2699.





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Validation

Rising bubble at different Péclet numbers



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Validation

Rising bubbles with different shapes

- Bubbles with generic shapes are corrected trough a shape factor: $Sr = {}^{A_{\Sigma}}/_{A_{sphere}}$
 - Four cases [*]:



* Farsoiya, P., Magdelaine, Q., Antkowiak, A., Popinet, S., & Deike, L. (2023). Direct numerical simulations of bubble-mediated gas transfer and dissolution in quiescent and turbulent flows. *Journal of Fluid Mechanics, 954,* A29.





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Taylor-Couette flow Flow instability and Taylor vortices

• Vortices enhance the mixing within the reactor







Taylor-Couette flow Flow instability and Taylor vortices

Vortices enhance the mixing within the reactor









Taylor-Couette flow Flow instability and Taylor vortices

Vortices enhance the mixing within the reactor







0.1

0.3

 $u_z/U_{\rm in}$

0.2

Taylor-Couette flow

Flow instability and Taylor vortices

- Contours of axial velocity at different Reynolds x
- Radius ratio $\eta = \frac{r_{in}}{r_{out}} = 0.5$
- Periodic top/bottom boundaries

Case	Re	Regime
a)	1000	Laminar
b)	3000	Turbulent
C)	5000	Turbulent



-0.3

-0.2

-0.1

0



Taylor-Couette flow

Flow instability and Taylor vortices

- $\times r_{\rm out})$ Contours of axial velocity at different Reynolds • z/(0.5
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Taylor-Couette flow Validation – Cylinder Torque

- Inner and Outer torques balance at equilibrium
- Non-dimensional torque:









Taylor-Couette flow Validation – Cylinder Torque







* Wendt, F. (1933). Turbulente strömungen zwischen zwei rotierenden konaxialen zylindern. Ingenieur-Archiv, 4(6), 577-595





Taylor-Couette flow Validation – Velocity field

Average azimuthal velocity







Taylor-Couette flow Validation – Velocity field

Average azimuthal velocity



Chouippe, A., Climent, E., Legendre, D., & Gabillet, C. (2014). Numerical simulation of bubble dispersion in turbulent taylor-couette flow. Physics of Fluids, 26 (4), 043304. Dong, S. (2007). Direct numerical simulation of turbulent taylor–couette flow. Journal of Fluid



Mechanics, 587, 373–393





Taylor-Couette flow Validation – Velocity field

- Average azimuthal velocity fluctuations
 - $-u_{\theta} = < u_{\theta} > + u_{\theta}'$
- Typical two-peak profiles near the walls (channel flow)



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Mass transfer in Taylor-Couette flow Simulation Setup

- A single bubble is let free to rise in an under-saturated liquid
- Ga = 1050.7, Bo = 3.4, Sc = 0.458, $\rho_c/\rho_d = 767.7$, $\mu_c/\mu_d = 52.2$

r _{out}	Case	Re	Regime	$D_b^{t=0}/d$	Cells/ $D_b^{t=o}$	Gravity
Tim	a)	0	N/A	1/3	164	yes
	b)	1000	Laminar	1/3	164	yes
	C)	3000	Turbulent	1/3	164	yes
	d)	5000	Turbulent	1/3	164	yes
	e)	1000	Laminar	1/3	164	no
	f)	3000	Turbulent	1/3	164	no
	g)	5000	Turbulent	1/3	164	no



Regime

Laminar

Turbulent

Turbulent

N/A



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Mass transfer in Taylor-Couette flow

Iso-surfaces of dissolved gas

 Iso-surfaces of dissolved gas r_{out} Case Re r_{in} a) 0 b) 1000 C) 3000 d) 5000

a)	
Re =	= 0





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Mass transfer in Taylor-Couette flow

Iso-surfaces of dissolved gas

 Iso-surfaces of dissolved gas r_{out} r_{in} 2

Case	Re	Regime
a)	0	N/A
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Mass transfer in Taylor-Couette flow

Iso-surfaces of dissolved gas

 Iso-surfaces of dissolved gas r_{out} r_{in}

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Re = 3000





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Mass transfer in Taylor-Couette flow

Iso-surfaces of dissolved gas

 Iso-surfaces of dissolved gas r_{out} r_{in} a b С d

Case	Re	Regime
)	0	N/A
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Mass transfer in Taylor-Couette flow

Volume dissolution

- Bubble initial diameter is 1/3 of the gap
- Buoyancy and surface tension overcome the effect of the carrier flow on the dissolution rate.







Sh -Mass transfer in Taylor-Couette flow Re_b — Sherwood numbers b) 40 1600 30 1200 Re_b Sh20 800 10 400 Re = 1000Re = 00 0 d 40160030

- $Sh = \frac{k_m D_b}{D}$, $k_m = -\frac{\int_{\Sigma} \dot{m} dS}{A_{\Sigma} M \Delta c}$ • $Re_b = \frac{\bar{\rho}_c U_b D_b}{\mu_c}$
- Sh and Re are generally related in bubbly flows driven by buoyancy.



t[s]

0,020,040,060,0°0,1

Re = 3000

Sh

20

10





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Mass transfer in Taylor-Couette flow Sherwood numbers

• Typical behavior of the Sh - Re curves suggests a comparison against common correlation formulae*:

$$-Sh = 2 + 0.651 \frac{Pe^{1.72}}{1 + Pe^{1.22}} \text{ for } Re_b \to 0, Sc \to \infty$$
$$-Sh = 2 + \frac{0.232Pe^{1.72}}{1 + 0.205Pe^{1.22}} \text{ for } Re_b \to \infty, Sc \to 0$$



Present work -

Mass transfer in Taylor-Couette flow Sherwood numbers

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Mass transfer in Taylor-Couette flow







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Taylor-Couette flow







Bottom bubble -

×

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July 6th, Pa Single bubble

Taylor-Couette flow Wake effect

- The top bubble behaves as if it were isolated
- The bottom bubble has a slower dissolution rate







Single bubble

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Taylor-Couette flow Wake effect

- The top bubble behaves as if it were isolated
- The bottom bubble has a slower dissolution rate
- For larger rotating speed (and stronger Taylor vortices), top and bottom bubbles behave similarly







Conclusions

- Numerical framework for the mass transfer of soluble species in two-phase incompressible flows based on Henry's law.
- Redistribution of the mass source term and divergence-free velocity field in interfacial cells.
- Modelling and Validation of laminar and turbulent Taylor-Couette flows
- Large bubbles are less sensitive to the carrier flow (in terms of dissolution rate)
- Standard Sh correlation formulae can provide sensible results when bubbles are mainly driven by gravity
- Stronger Taylor vortices generate more dispersion and enhance global mass transfer for multiple bubbles

Thank you for your attention Any questions?