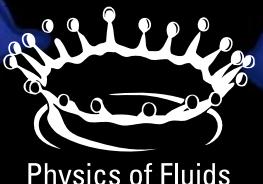


Laboratoire de Mécanique des Fluides de Lille (LMFL)

Heat and mass transport in porous media: Insights from experiments, simulations, and modelling



M. De Paoli^{1,2}

m.depaoli@utwente.nl

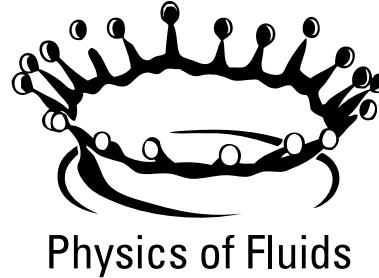
¹Physics of Fluids Group, University of Twente, Enschede (The Netherlands)

²Institute of Fluid Mechanics and Heat Transfer, TU Wien, Vienna (Austria)



Acknowledgements

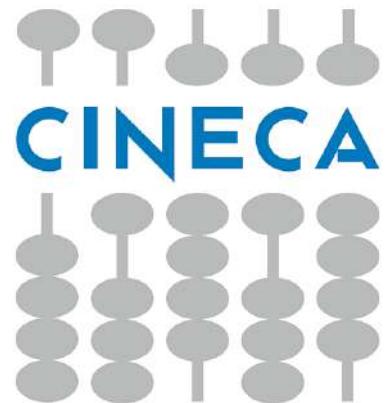
UNIVERSITY OF TWENTE.



Marie Skłodowska-Curie postdoctoral fellowship No. 101062123.

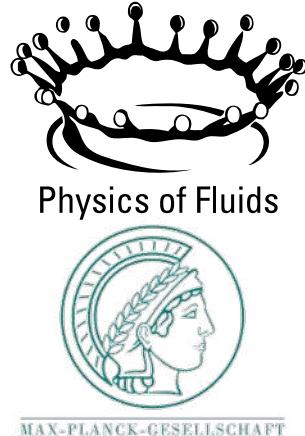


Erwin Schrödinger postdoctoral fellowship No. J-4612



EuroHPC
Joint Undertaking

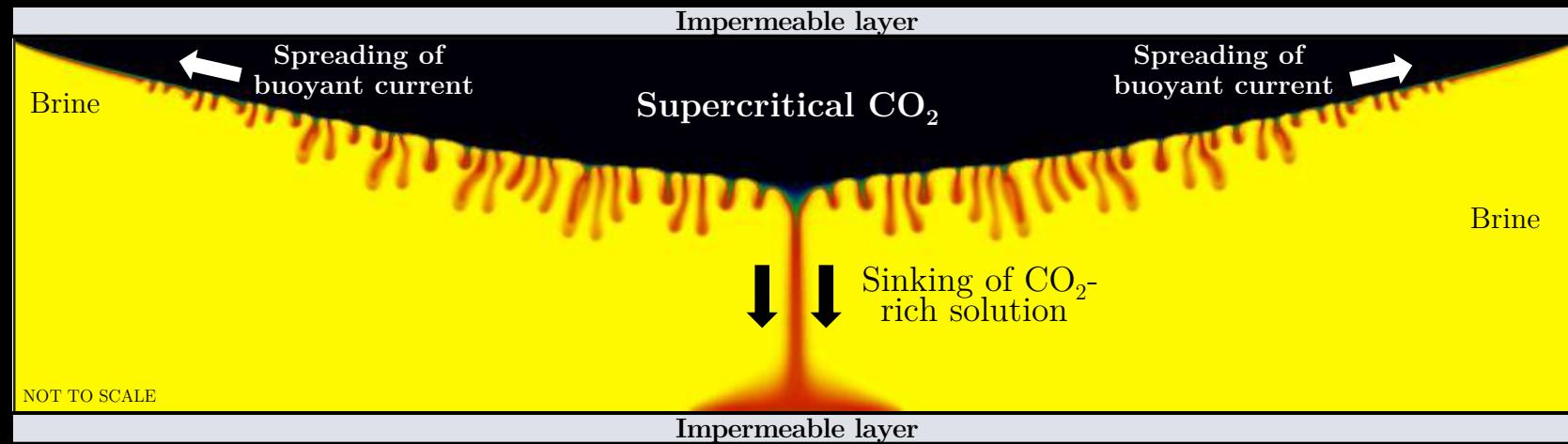
Acknowledgements



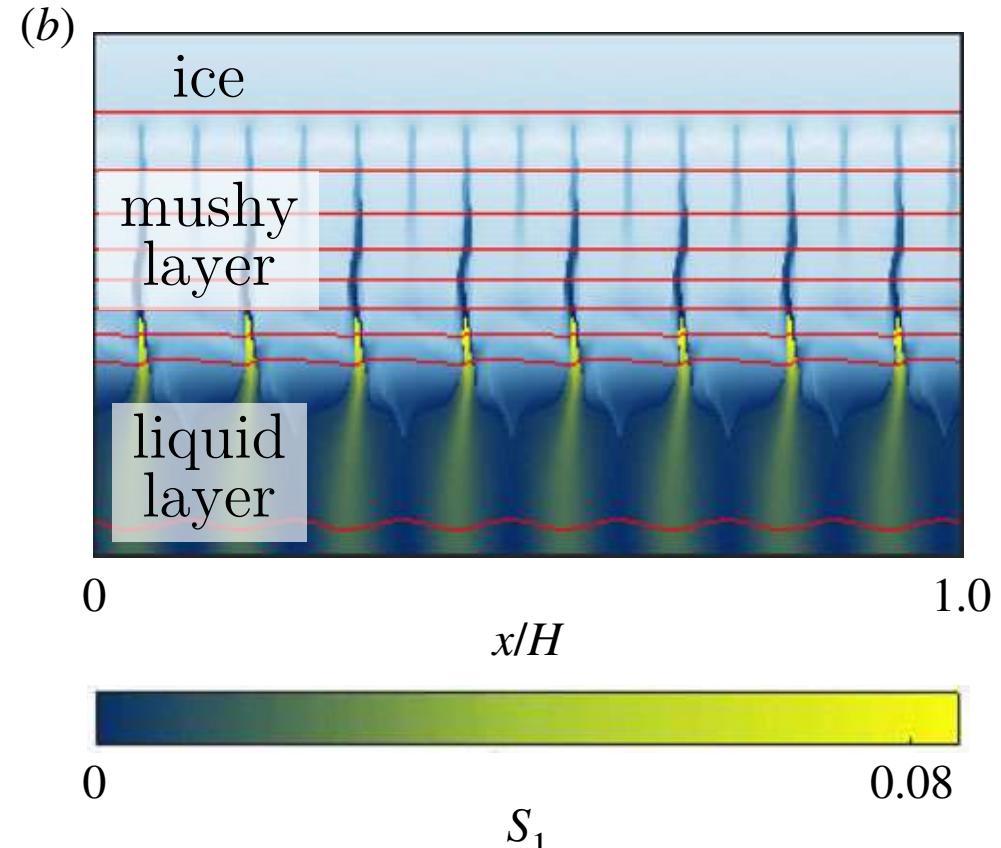
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2. Reservoir-scale: multiphase gravity currents
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Sea ice formation



Wells AJ, Hitchen JR, Parkinson JRG., «Mushy-layer growth and convection, with application to sea ice» 2019 *Phil. Trans. R. Soc. A*

Middleton et al., “Visualizing brine channel development and convective processes during artificial sea-ice growth using Schlieren optical methods”. *J. Glaciology* (2016).

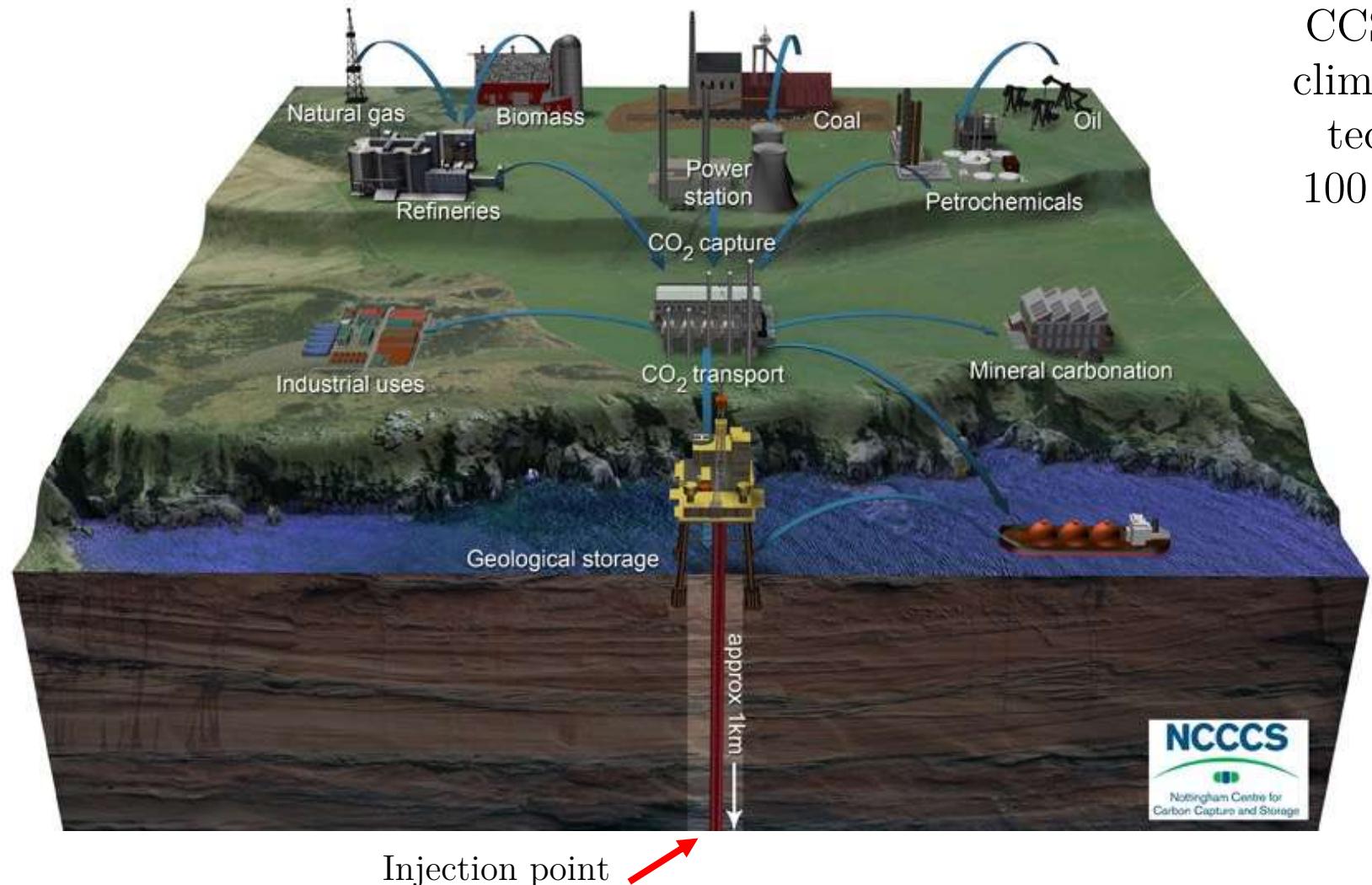
Other applications

Simmons et al., “Variable-density groundwater flow and solute transport in heterogeneous porous media: approaches, resolutions and future challenges,” *J. Contam. Hydrol.* (2001).

Molen et al., “Transport of solutes in soils and aquifers,” *J. Hydrol.* (1988).

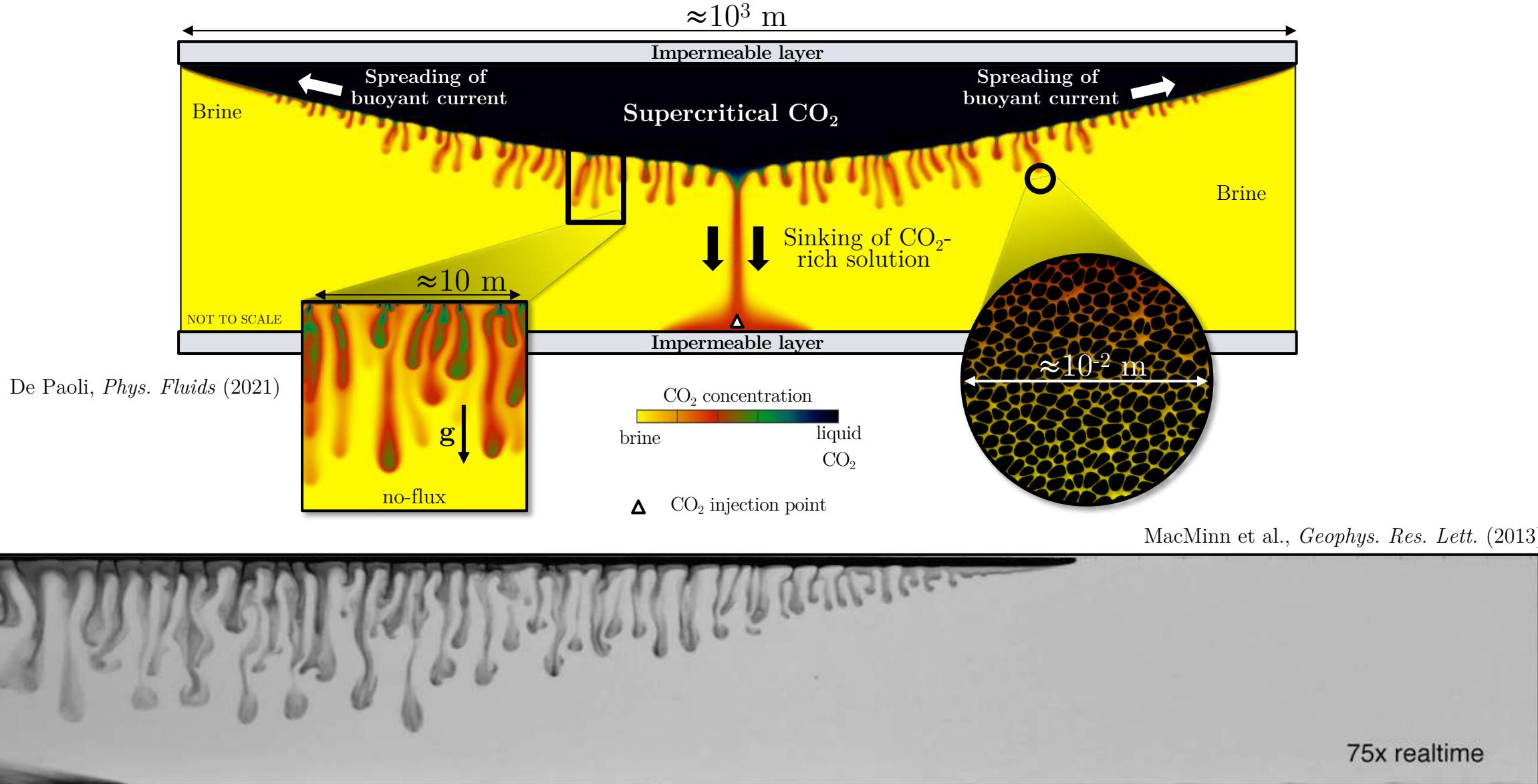
LeBlanc, *Sewage plume in a sand and gravel aquifer, Cape Cod, Massachusetts* (US Geological Survey, 1984).

Carbon Capture and Storage (CCS)

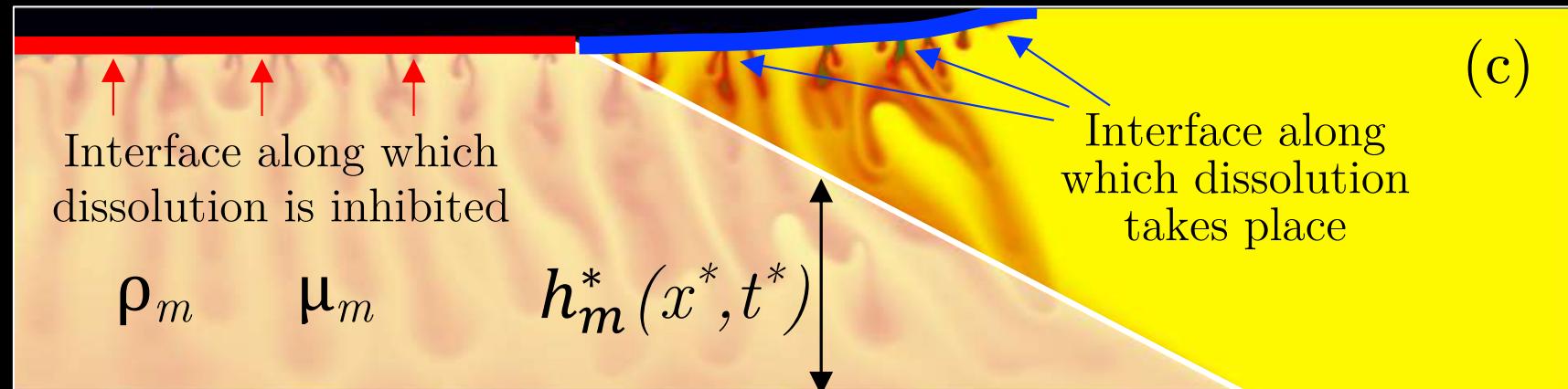


CCS can work as unique climate change mitigation technology for at least 100 years [Szulczewski *et al.*, (PNAS) 2012]

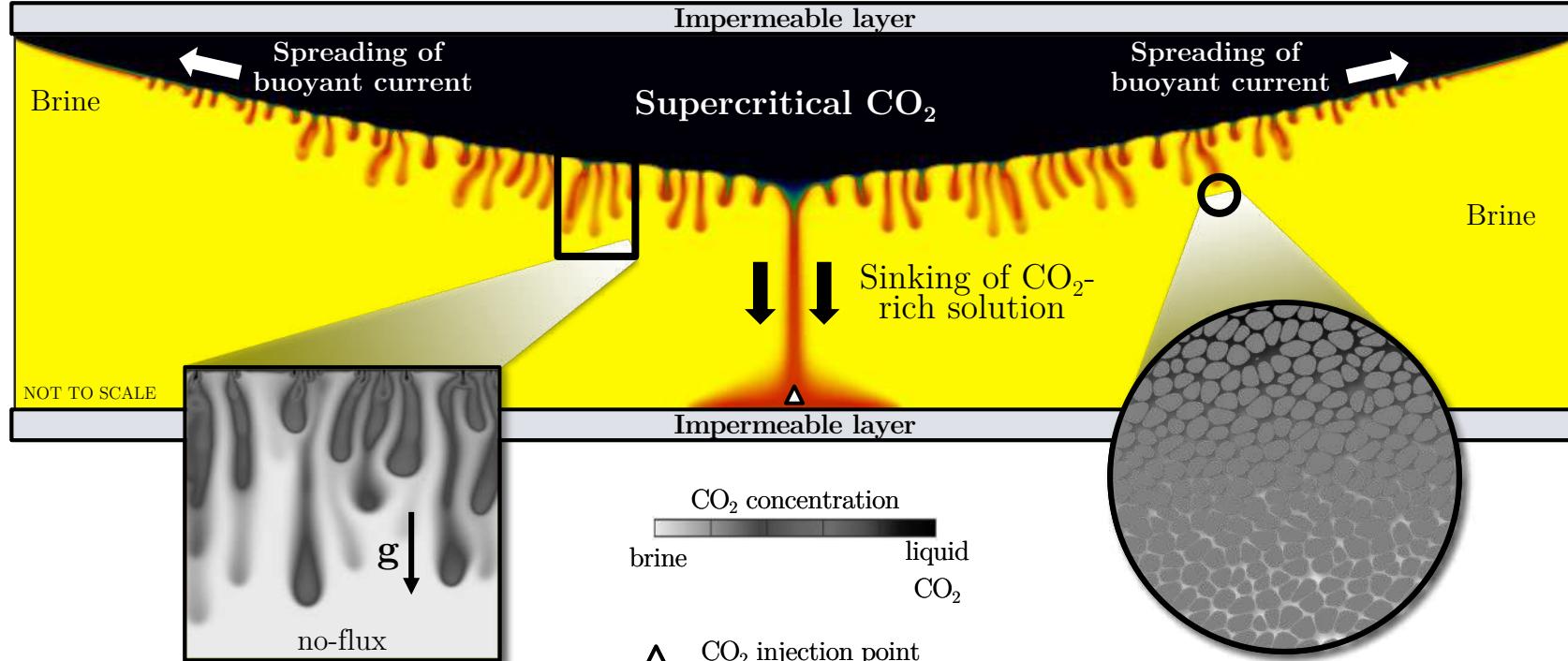
Carbon Capture and Storage



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Carbon Capture and Storage

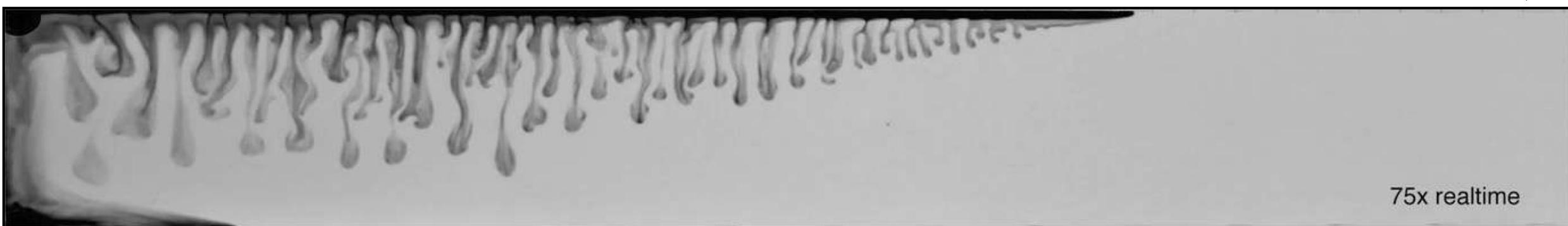


De Paoli, *Phys. Fluids* (2021)

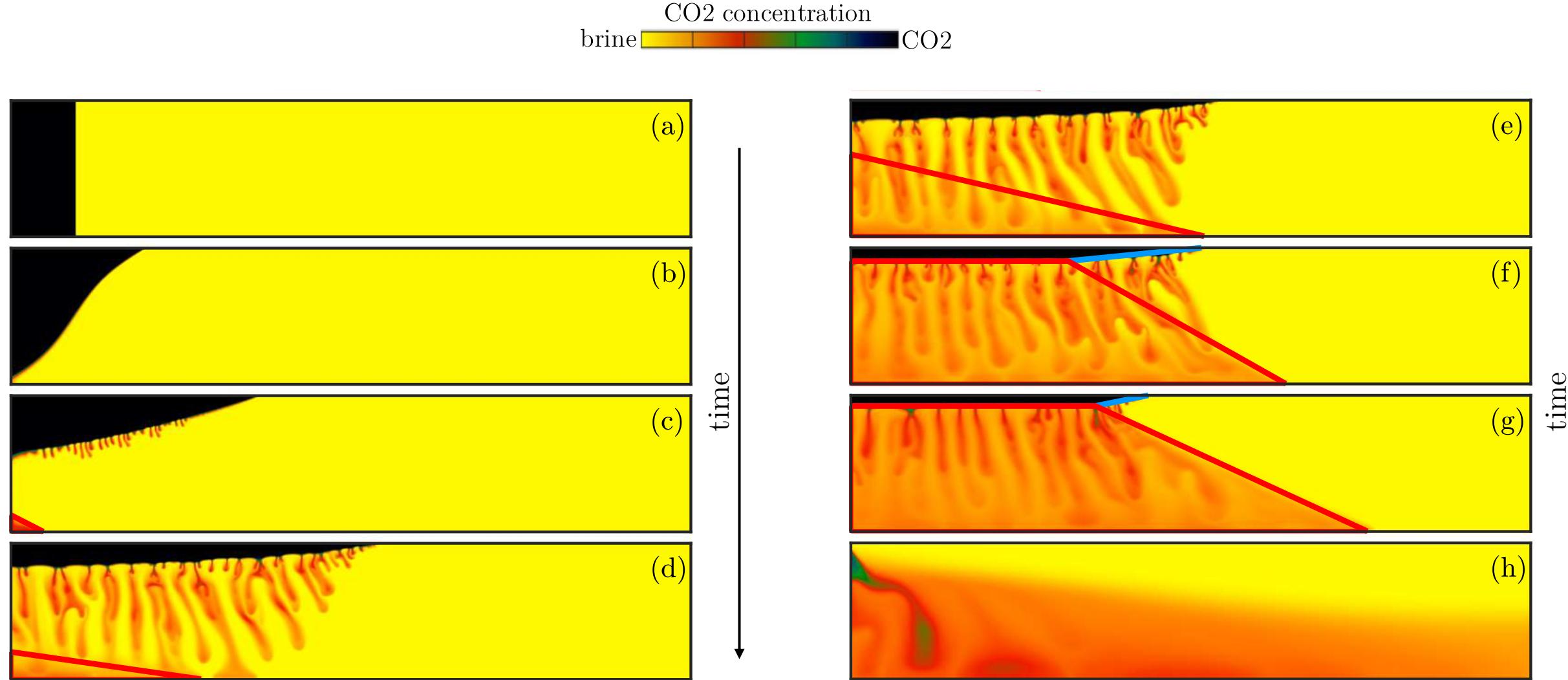
Reservoir properties

- anisotropy and heterogeneities
- finite size of confining layers
- effects of rock properties (mechanical dispersion)
- chemical dissolution and morphology variations
- ...

MacMinn & Juanes., *Geophys. Res. Lett.* (2013)

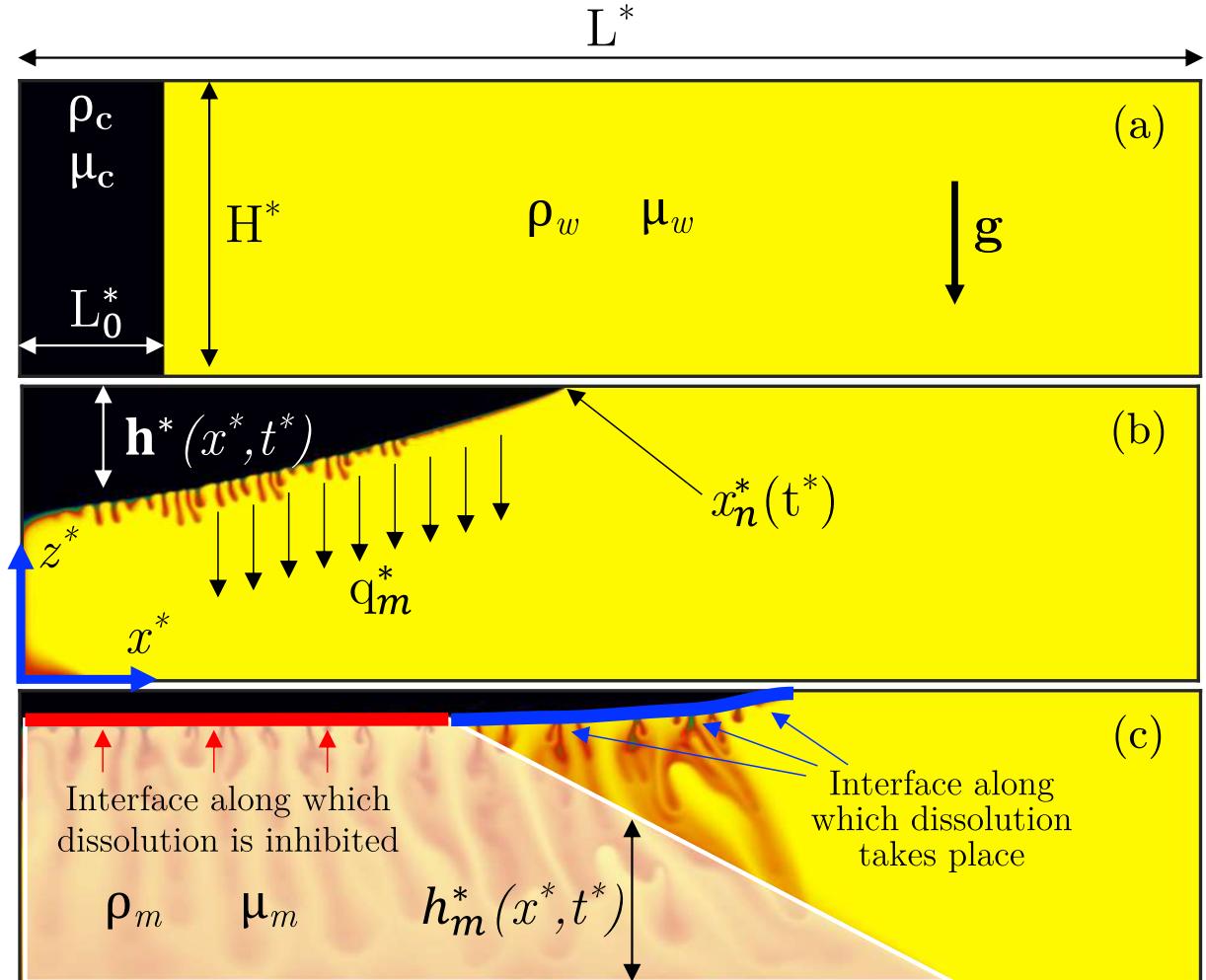


Multiphase gravity currents with dissolution



De Paoli, *Phys. Fluids.* (2021)

Multiphase gravity currents with dissolution



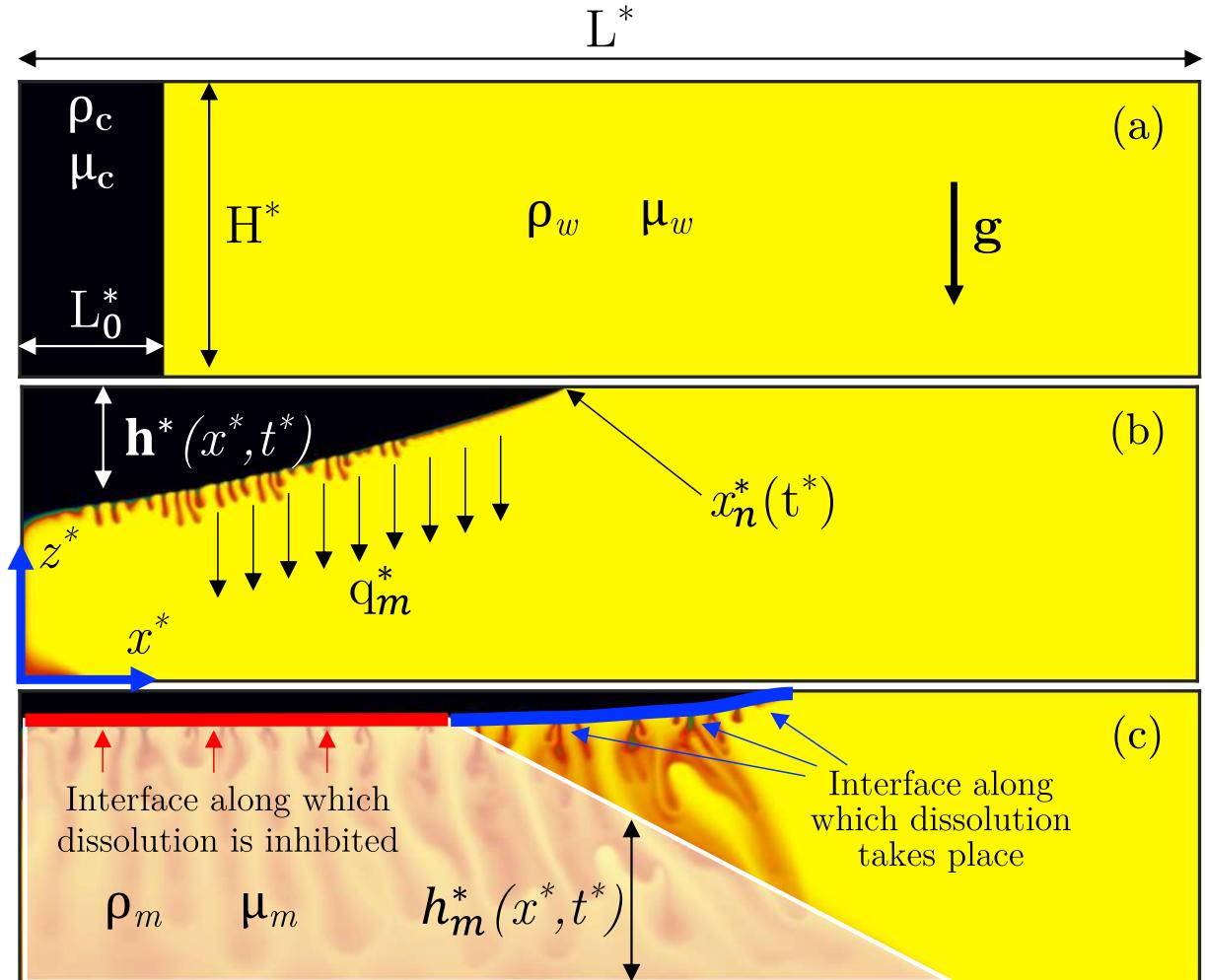
$$\nabla \cdot \mathbf{u}_i^* = 0$$

$$\mathbf{u}_i^* = \frac{1}{\mu_i} \mathbf{K}(-\nabla p_i^* + \rho_i \mathbf{g})$$

$$\phi \frac{\partial C^*}{\partial t^*} + \mathbf{u}_i^* \cdot \nabla C^* = \phi \nabla \cdot [\mathbf{D}(\mathbf{u}_i^*) \cdot \nabla C^*]$$

De Paoli, *Phys. Fluids.* (2021)

Multiphase gravity currents with dissolution



$$\frac{\partial h}{\partial t} - \frac{\partial}{\partial x} \left[(1-f)h \frac{\partial h}{\partial x} - \delta f h_m \frac{\partial h_m}{\partial x} \right] = -\varepsilon_0,$$

$$\frac{\partial h_m}{\partial t} - \frac{\partial}{\partial x} \left[\delta(1-f_m)h_m \frac{\partial h_m}{\partial x} - f_m h \frac{\partial h}{\partial x} \right] = \frac{\varepsilon_0}{X_v}$$

$$f = \frac{Mh^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

$$f_m = \frac{M_mh_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

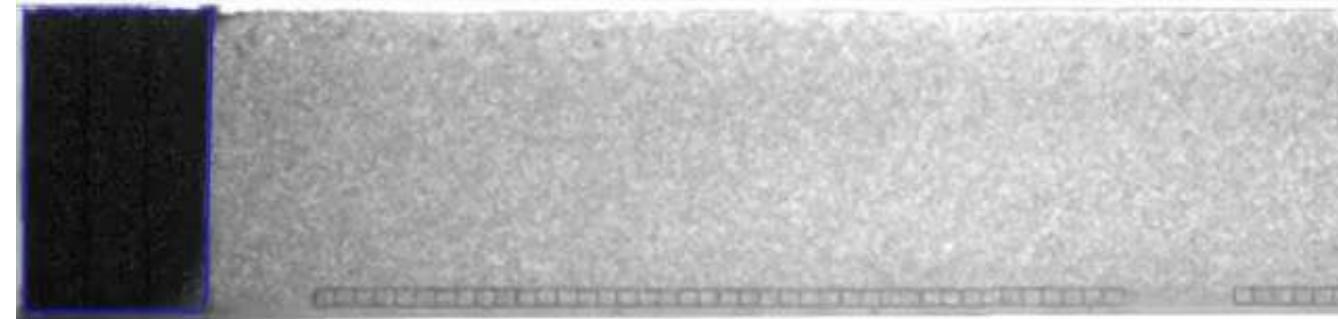
MacMinn, Neufeld, Hesse,
and Huppert, *Water Resour. Res.* (2012)

Mobility ratios $M = \mu_w/\mu_c$ and $M_m = \mu_w/\mu_m$

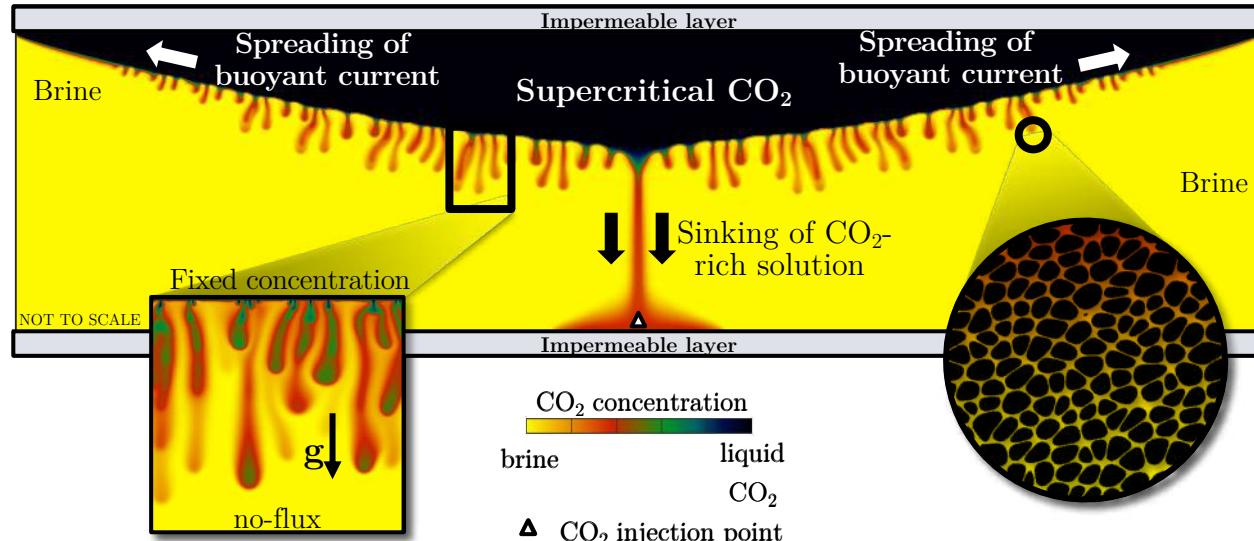
Buoyancy velocity ratio $\delta = W_m^*/W^*$

Volume fraction $X_v = \rho_m X_m / \rho_c$

Multiphase gravity currents with dissolution



MacMinn, Neufeld, Hesse, and Huppert, *Water Resour. Res.* (2012)



$$\frac{\partial h}{\partial t} - \frac{\partial}{\partial x} \left[(1-f)h \frac{\partial h}{\partial x} - \delta f h_m \frac{\partial h_m}{\partial x} \right] = -\varepsilon_0,$$

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$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

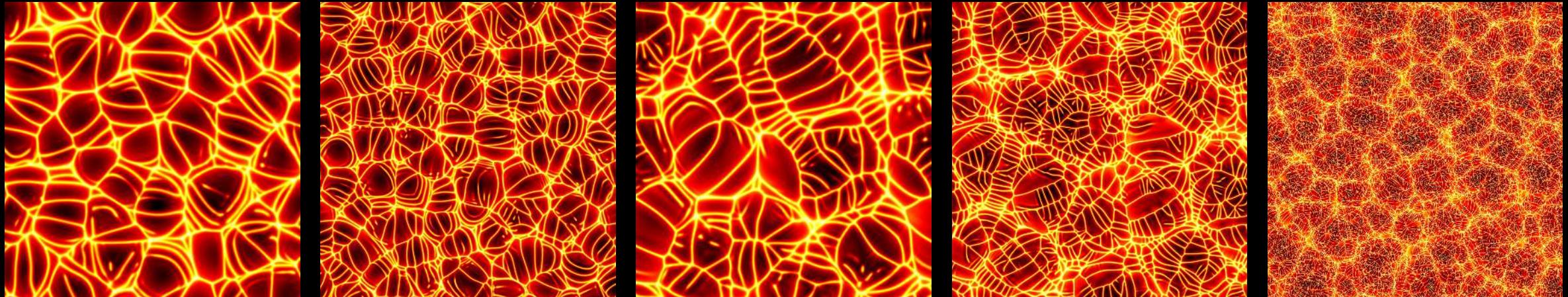
$$\varepsilon_0(x) = \begin{cases} 0 & \text{if } h(x) = 0 \text{ or } h(x) + h_m(x) = 1 \\ \varepsilon & \text{else,} \end{cases}$$

$$\varepsilon = \frac{q_m^*}{\phi W^*} \left(\frac{L_0^*}{H^*} \right)^2$$

How to determine the dissolution rate q_m^* ?

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Dimensionless equations

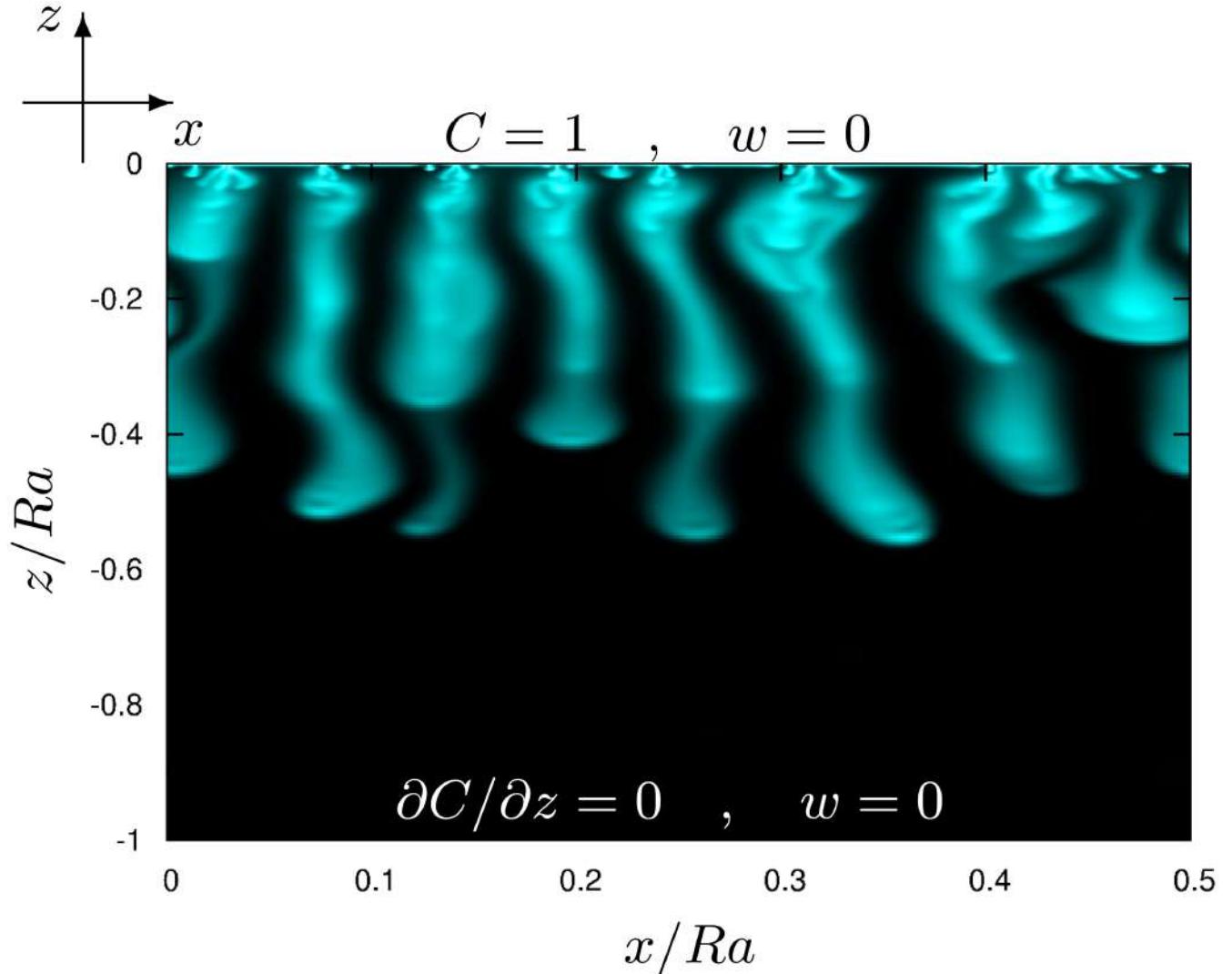
$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + w \frac{\partial C}{\partial z} = \frac{1}{Ra} \left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2} \right)$$

$$u = -\frac{\partial P}{\partial x} \quad , \quad w = -\frac{\partial P}{\partial z} - C$$

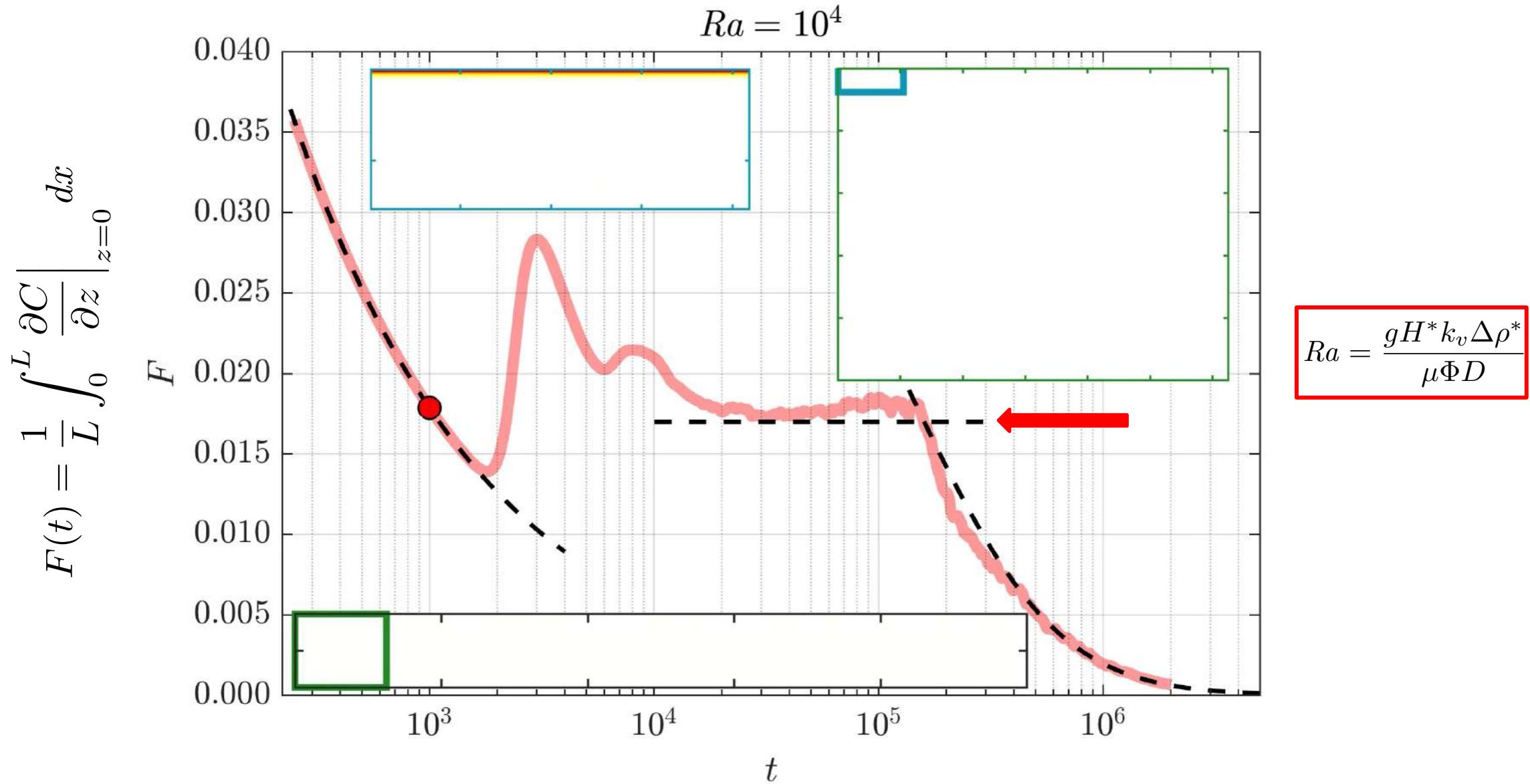
$$\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} = 0$$

Governing parameter

$$Ra = \frac{g H^* k_v \Delta \rho^*}{\mu \Phi D}$$



Convective dissolution process



Convection in anisotropic media

Examples of model extension:
effect of **anisotropy** of the medium



benedek / Getty Images

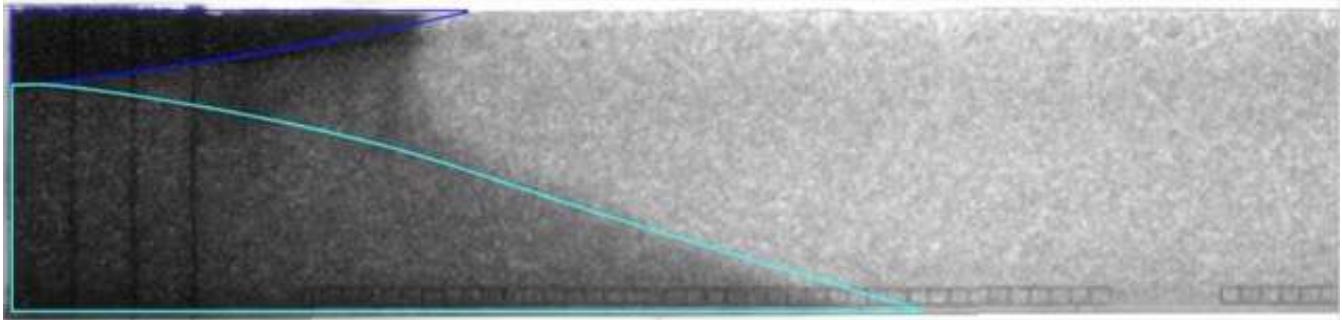
In this presentation we just consider the anisotropy of the rocks, for additional effects (lateral confinement, dispersion) see De Paoli, *Phys. Fluids* (2021)

Sedimentary rocks: Rocks formed by stratification

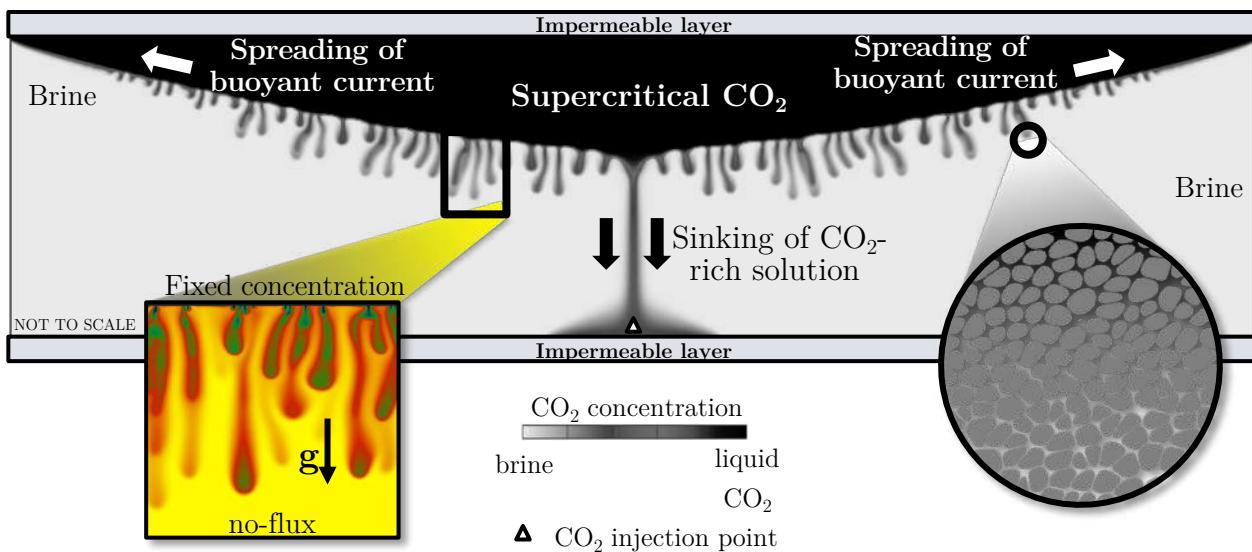


Rhododendrites/Wikimedia Commons/CC BY 4.0

Gravity currents with dissolution



MacMinn, Neufeld, Hesse, and Huppert, *Water Resour. Res.* (2012)



$$\frac{\partial h}{\partial t} - \frac{\partial}{\partial x} \left[(1-f)h \frac{\partial h}{\partial x} - \delta f h_m \frac{\partial h_m}{\partial x} \right] = -\varepsilon_0,$$

$$\frac{\partial h_m}{\partial t} - \frac{\partial}{\partial x} \left[\delta(1-f_m)h_m \frac{\partial h_m}{\partial x} - f_m h \frac{\partial h}{\partial x} \right] = \frac{\varepsilon_0}{X_v}$$

$$f = \frac{Mh^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

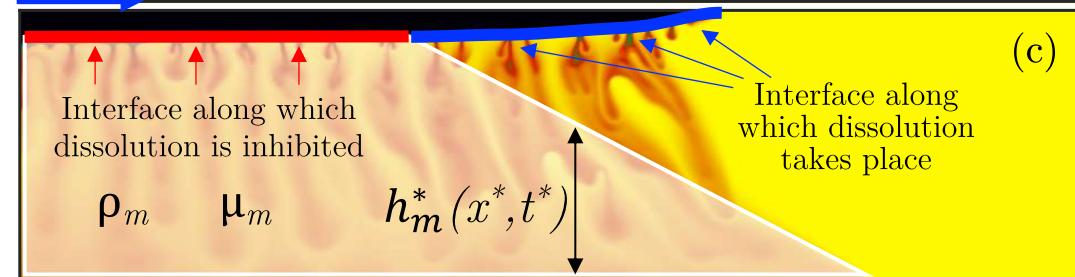
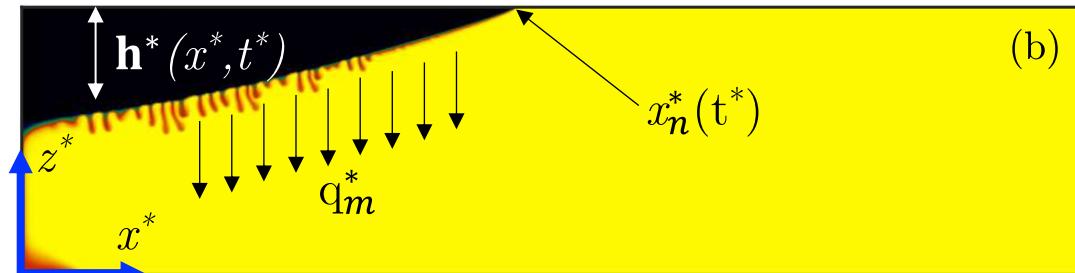
$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

$$\varepsilon_0(x) = \begin{cases} 0 & \text{if } h(x) = 0 \text{ or } h(x) + h_m(x) = 1 \\ \varepsilon & \text{else,} \end{cases}$$

$$\varepsilon = \frac{q_m^*}{\phi W^*} \left(\frac{L_0^*}{H^*} \right)^2$$

How to determine the dissolution rate q_m^* ?

Effect of anisotropy



Darcy-scale simulations:



$$\text{dissolution rate } q_m^* \sim \gamma^{-\frac{1}{2}}$$



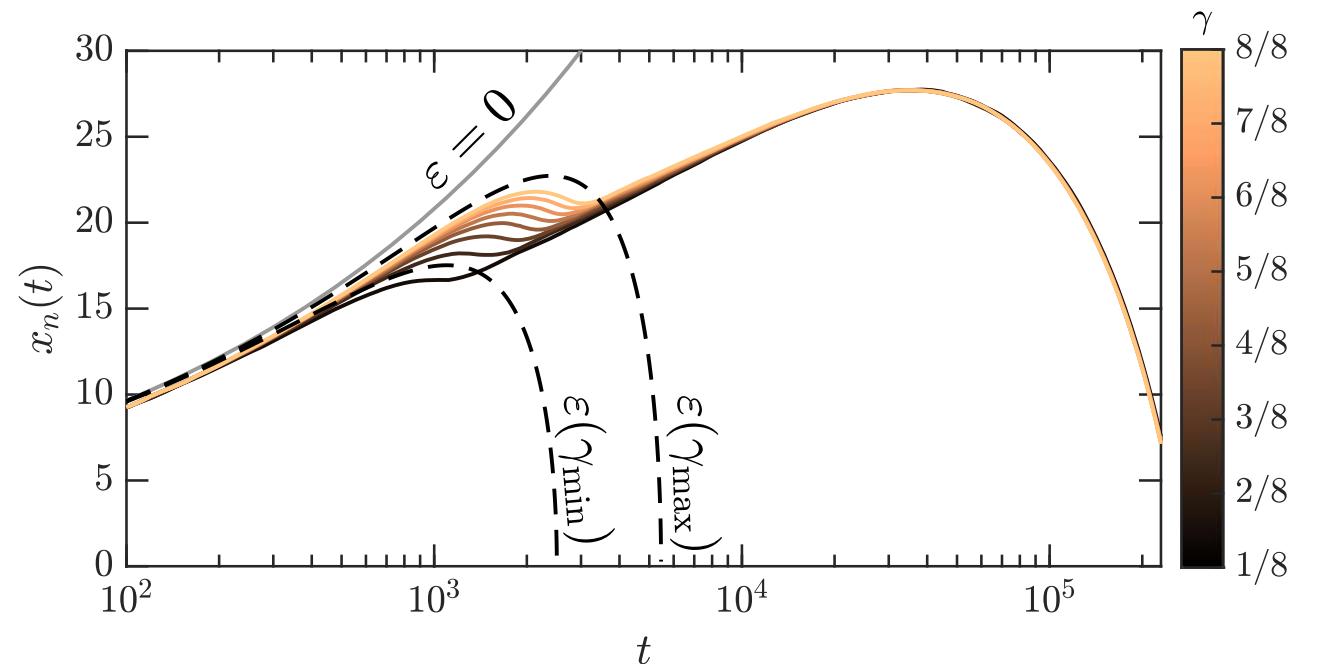
dissolution increases with the anisotropy of the medium

Sedimentary rocks are anisotropic

$$\gamma = \frac{k_v}{k_h} < 1$$

$\gamma = 1$ isotropic

$\gamma = 1/8$ strongly anisotropic



Analytical solution in case of

- no-dissolution —————
- independent currents -----

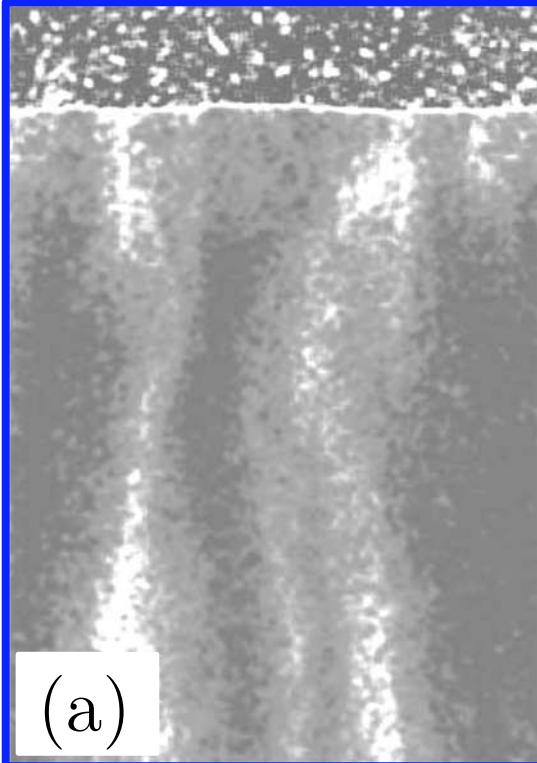
Scalings of convection and finite-size effect

Theory: linear scaling $Sh = F Ra \sim Ra$ is expected (see review of Hewitt, 2020)

Porous media experiments: $Sh \sim Ra^\alpha, \alpha < 1$ (Neufeld et al., *Geophys. Res. Lett.* 2010)

Hele-Shaw experiments: $Sh \sim Ra^\alpha, \alpha < 1$ (Backhaus et al., *Phys. Rev. Lett.* 2011)

Darcy simulations: $Sh \sim Ra$ (Hidalgo et al., *Phys. Rev. Lett.* 2012)

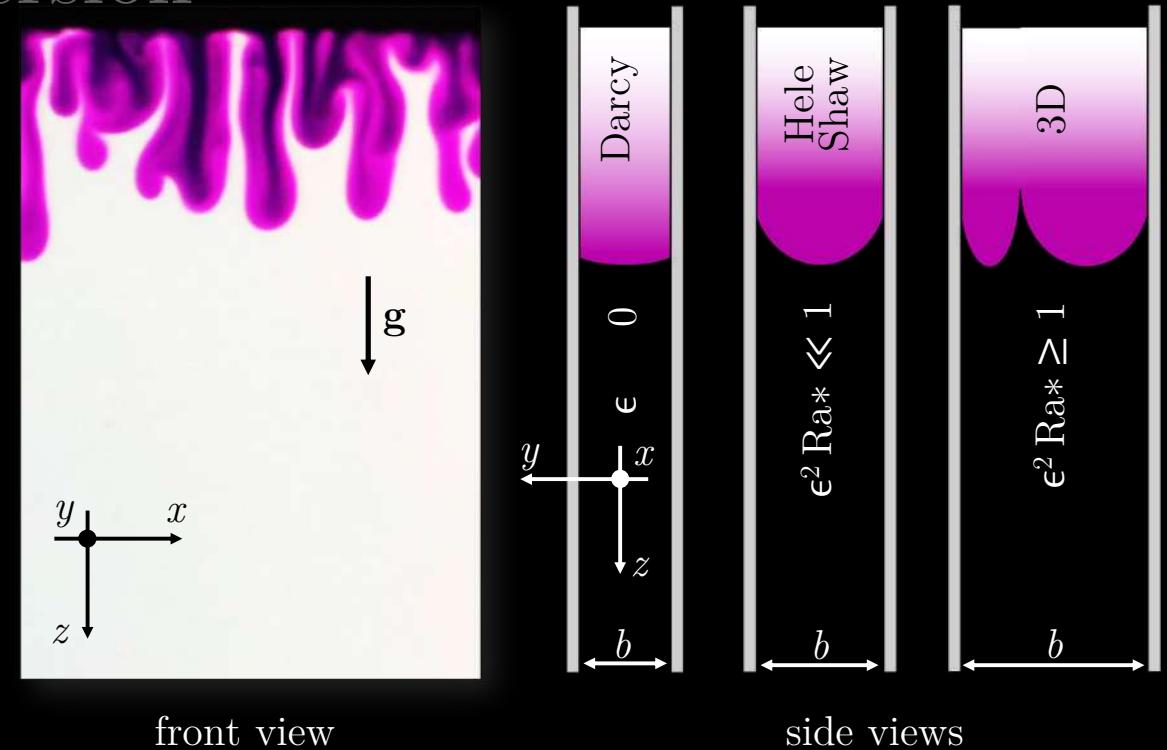


Differences arise due to effects not present in the Darcy model: consequences for **porous media** and **Hele-Shaw**

See De Paoli, *Eur. Phys. J. E* (2023) for a detailed discussion

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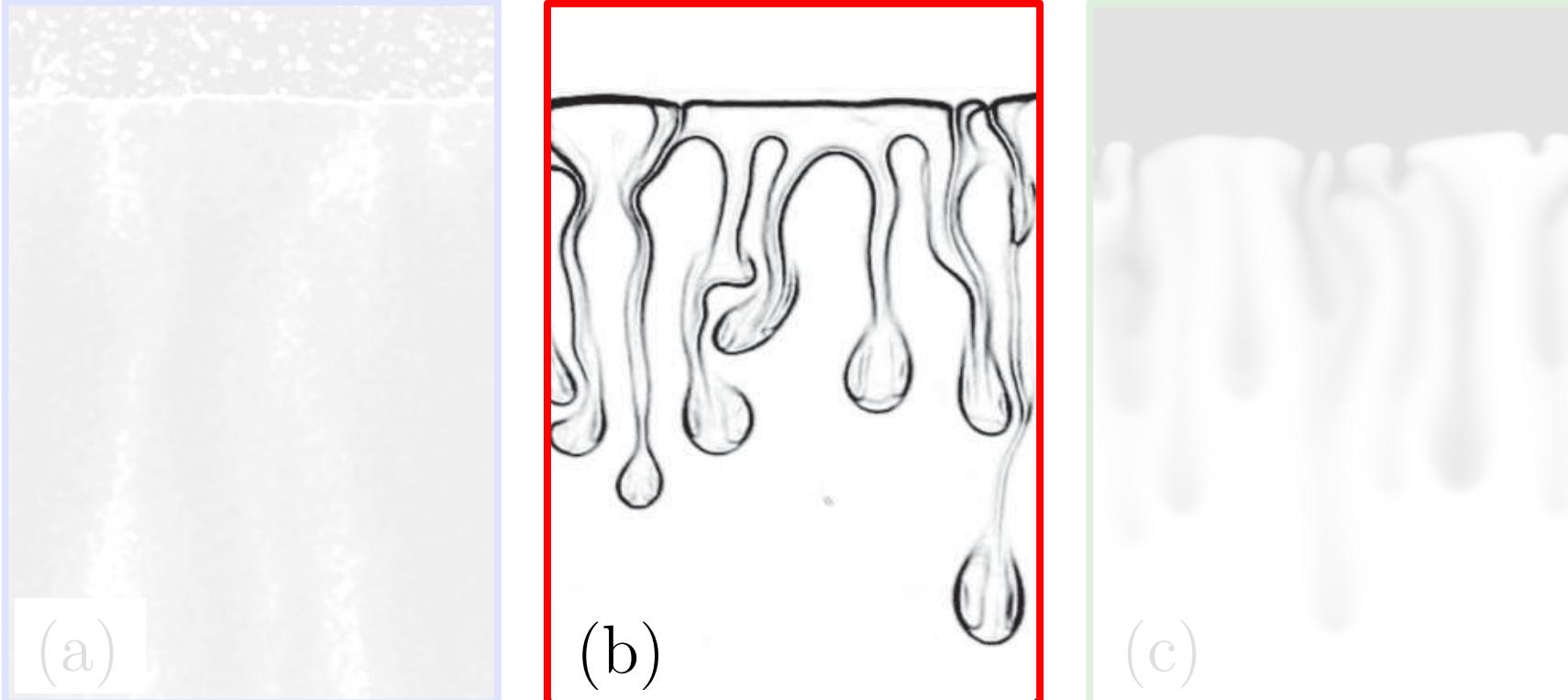
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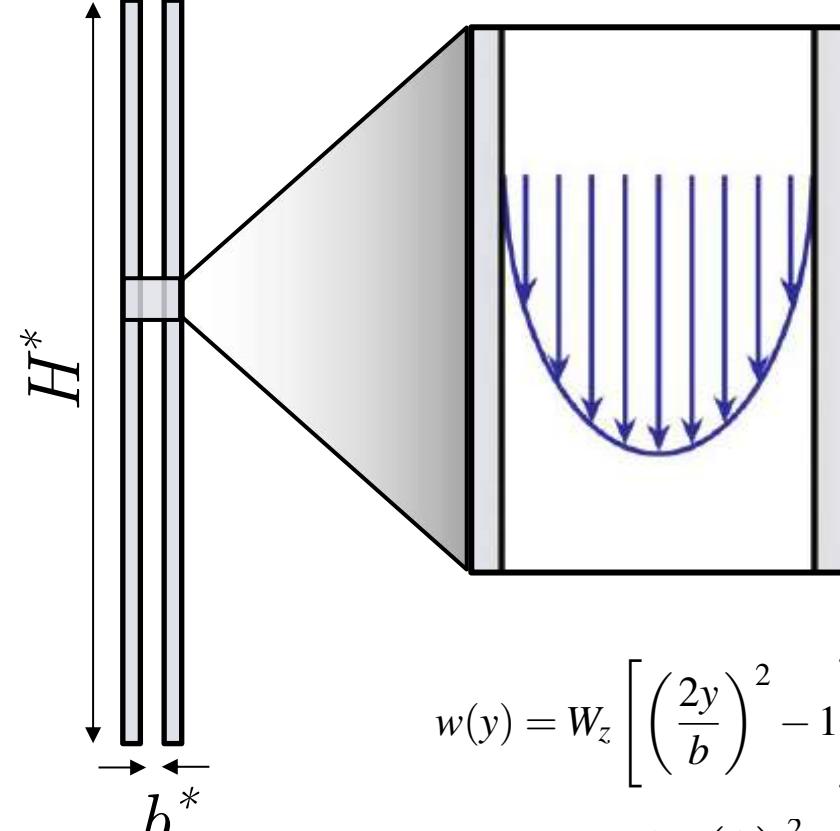
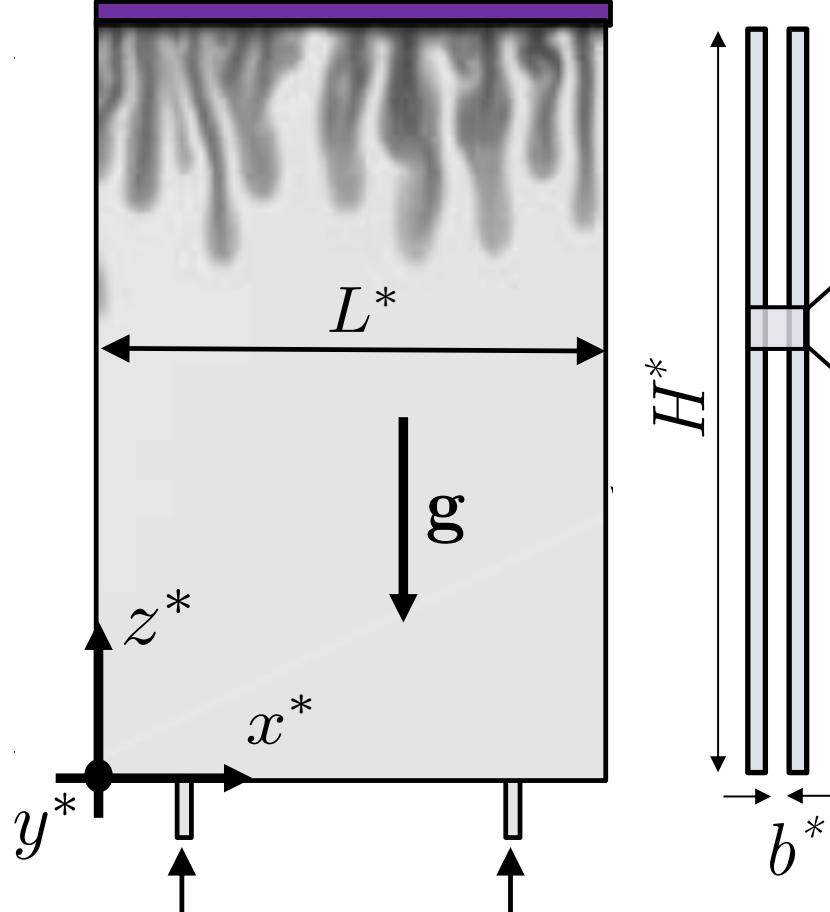
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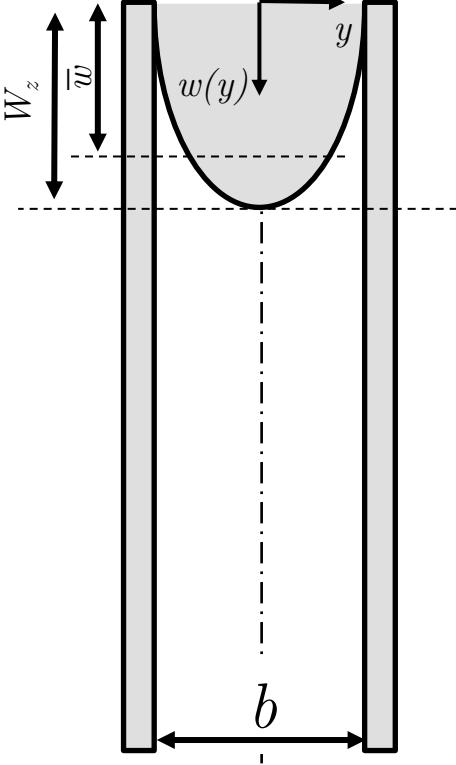
Experiments in Hele-Shaw cells



$$w(y) = W_z \left[\left(\frac{2y}{b} \right)^2 - 1 \right]$$

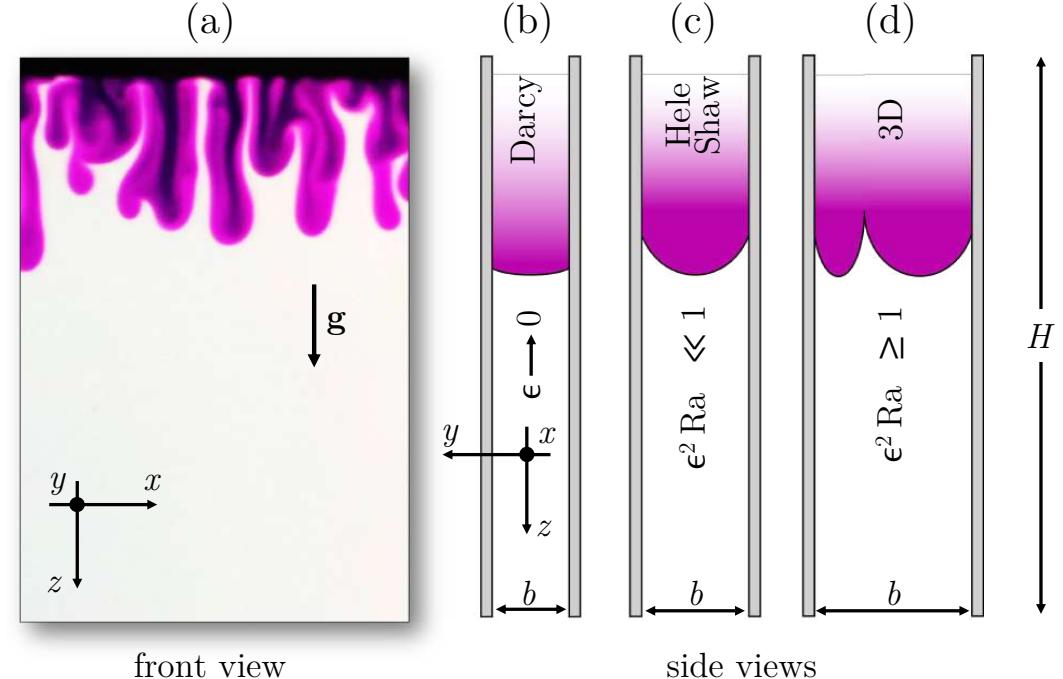
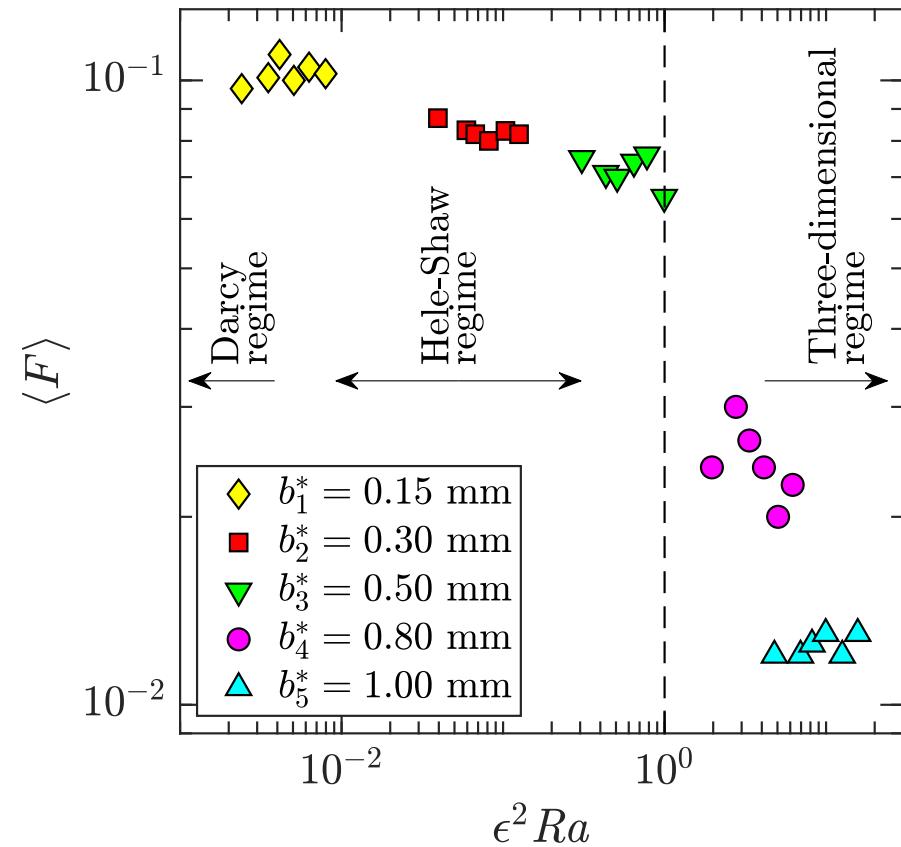
$$W_z = \frac{1}{2\mu} \frac{dp}{dz} \left(\frac{b}{2} \right)^2$$

$$\bar{w} = \frac{2}{3} W_z = \frac{b^2/12}{\mu} \left| \frac{dp}{dz} \right|$$



Alipour, De Paoli and Soldati, *Exp. Fluids* (2020)
 De Paoli, Alipour and Soldati, *J. Fluid Mech.* (2020)

Experiments in Hele-Shaw cells

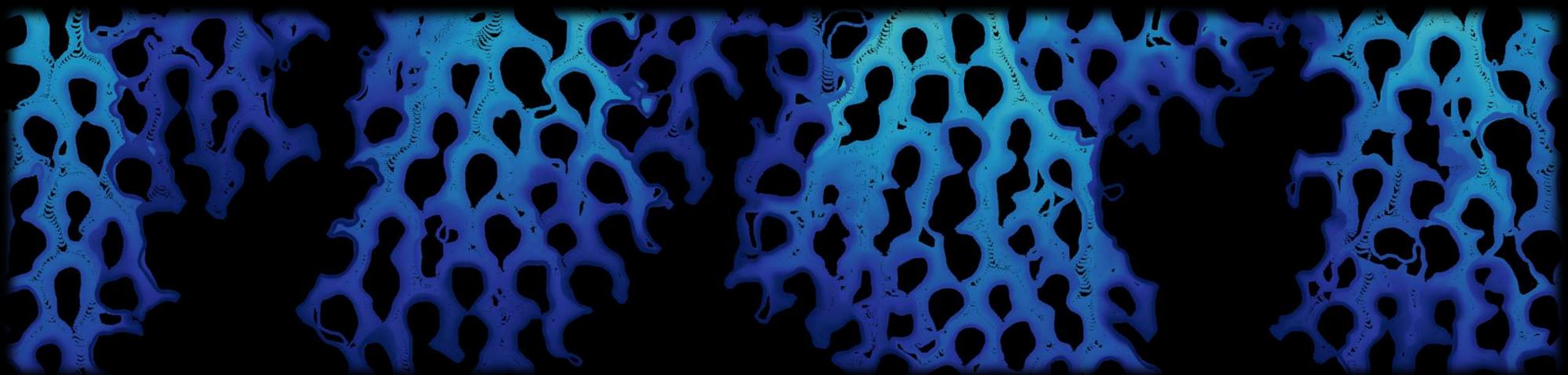


$$\epsilon^2 Ra \begin{cases} \rightarrow 0 \Rightarrow \text{Darcy flow} \\ \ll 1 \Rightarrow \text{Hele-Shaw flow} \\ > 1 \Rightarrow \text{three-dimensional} \end{cases}$$

This model has been further developed in
 Letelier *et al.*, *J. Fluid Mech.* (2023)
 Ulloa & Letelier, *J. Fluid Mech.* (2022)

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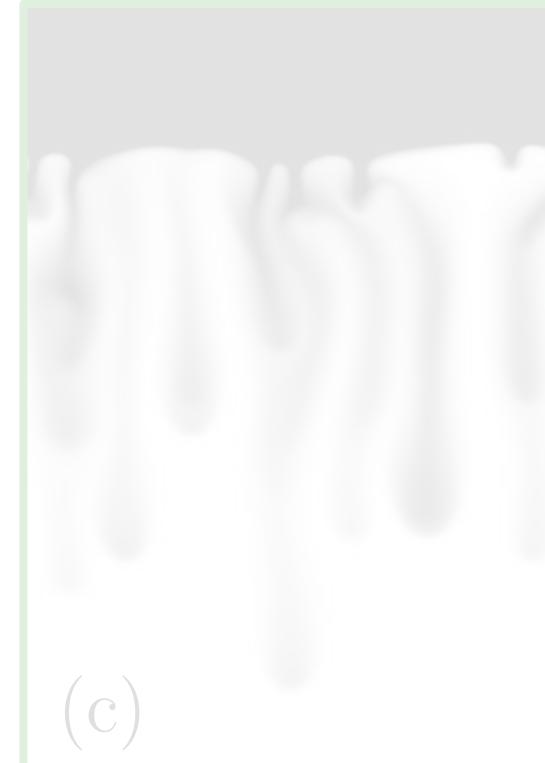
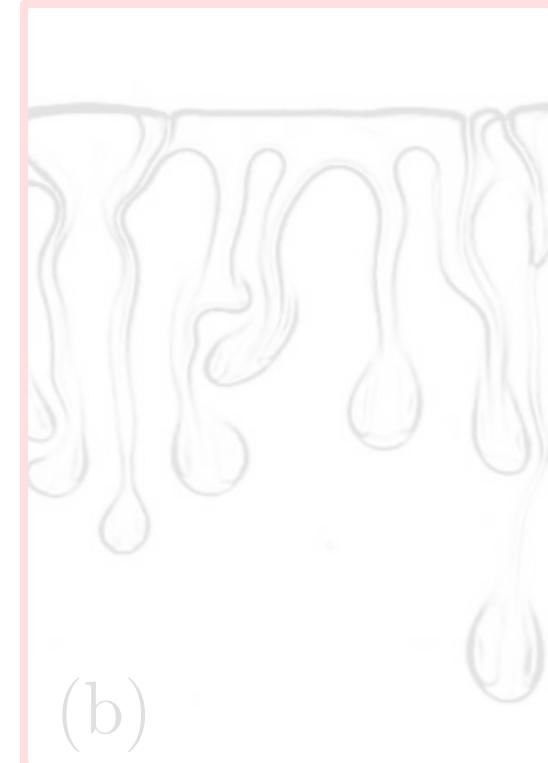
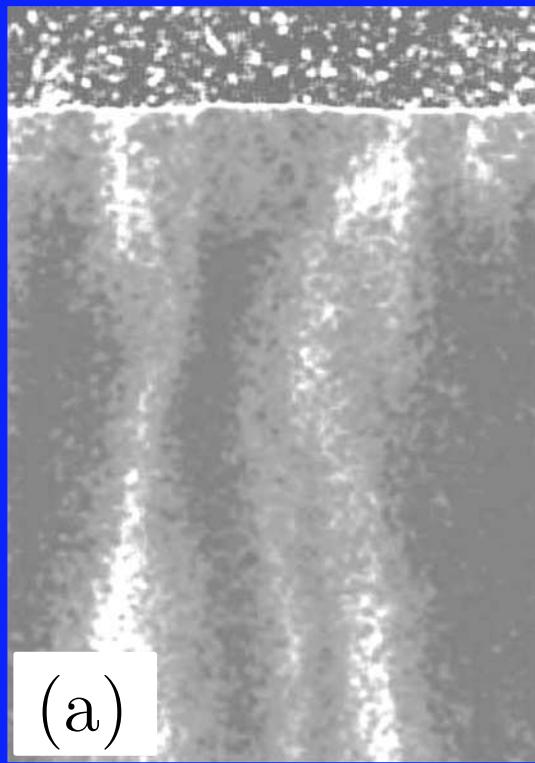
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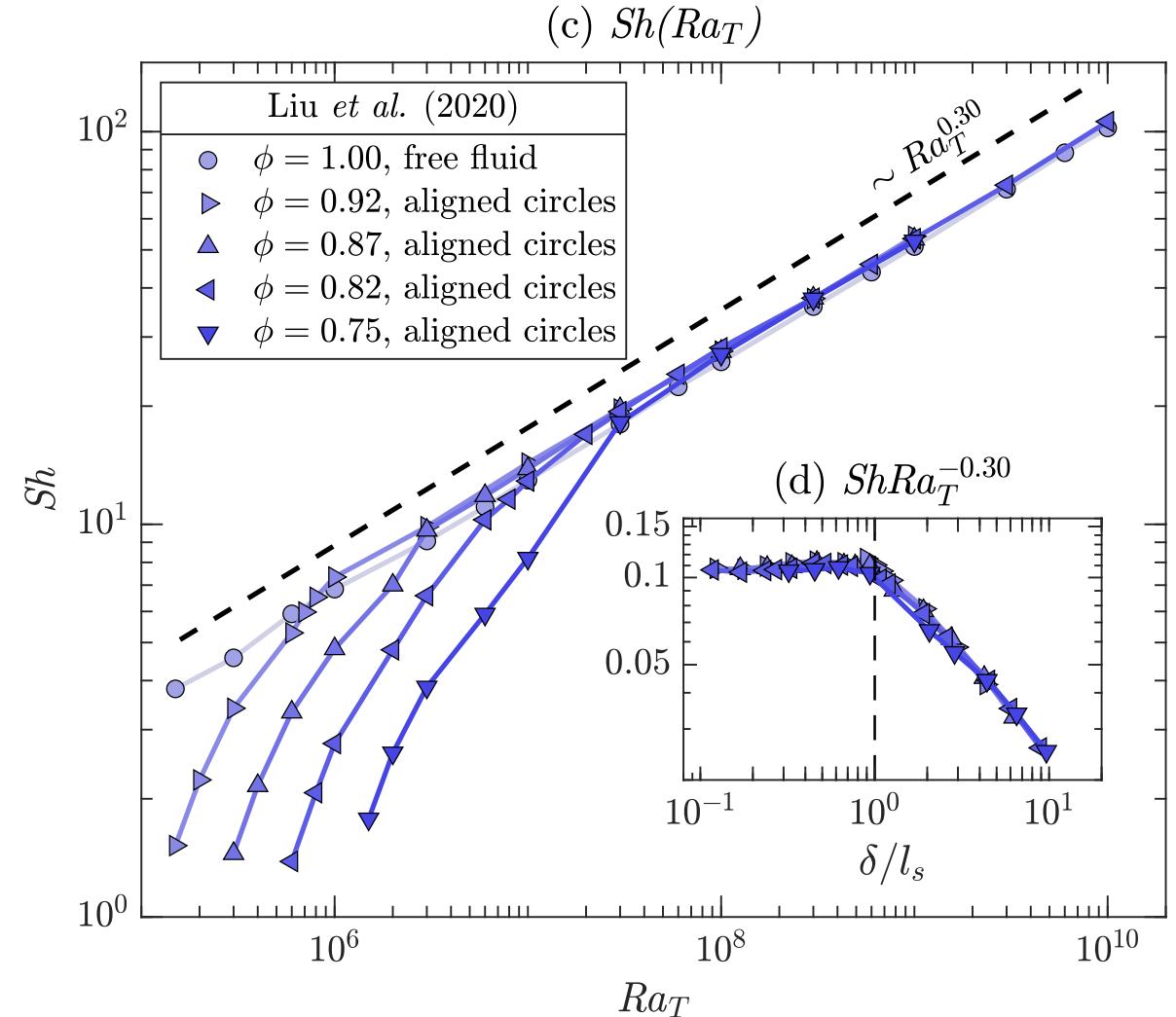
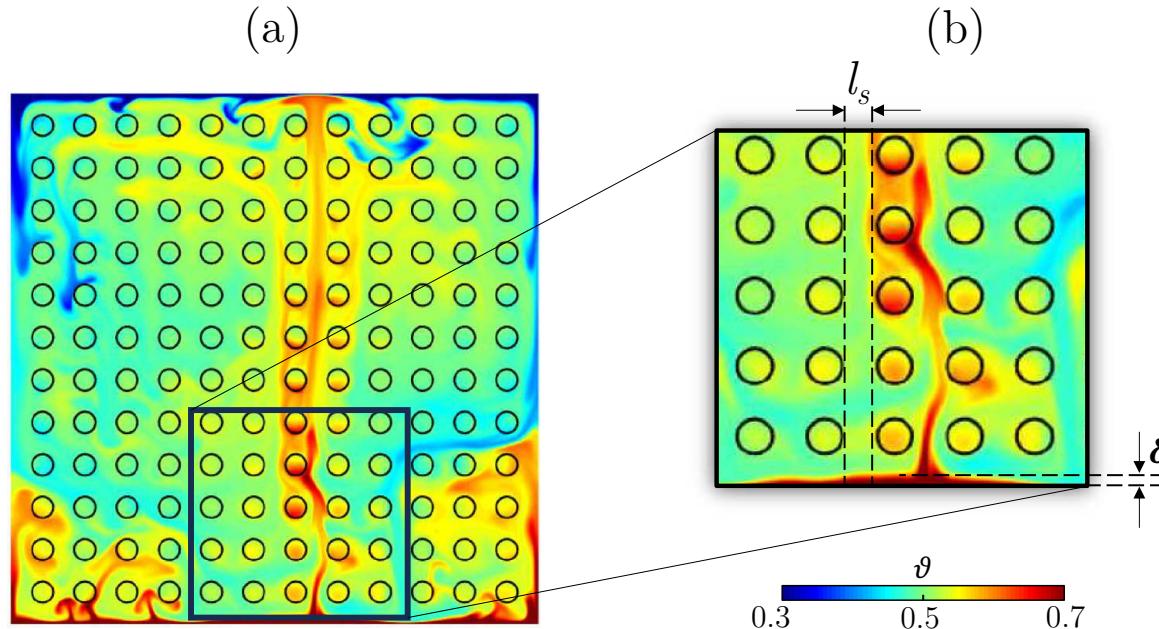


Differences arise due to effects not present in the Darcy model: consequences for **porous media** and **Hele-Shaw**

See De Paoli, *Eur. Phys. J. E* (2023) for a detailed discussion

Pore-scale simulations

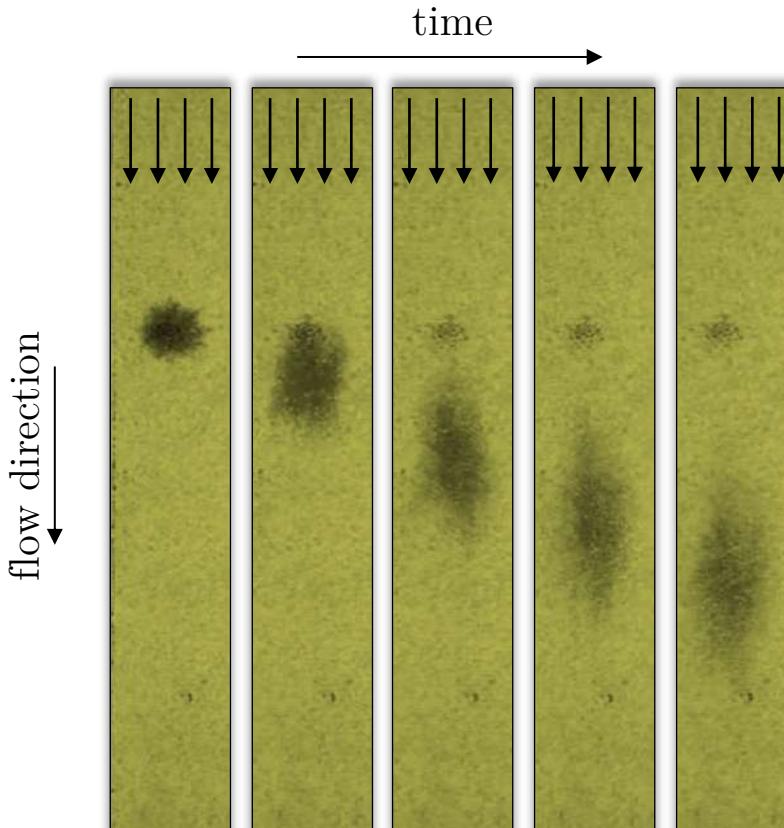
Additional non-Darcy effects:
Relative size of flow structures and pores



Influence of dispersion

Mechanism of dispersion

Patch of dye in a uniform flow through a porous medium



Woods, *Flows in porous rocks* (2015)

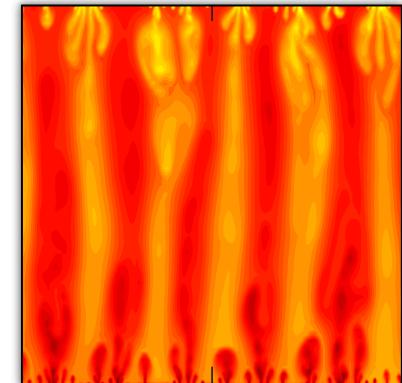
Darcy formulation of dispersion

$$\phi \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C - \phi D \nabla C) = 0$$

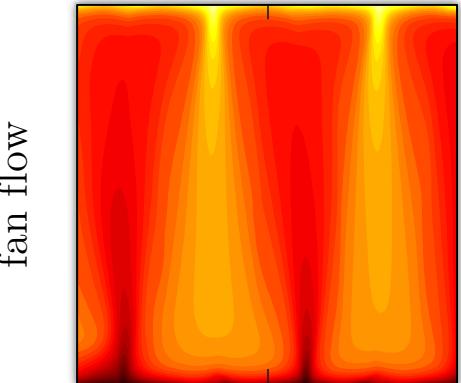
Fickian formulation for dispersion

$$\mathbf{D} = D\mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{u}\mathbf{u}}{|\mathbf{u}|} + \alpha_T \mathbf{u}\mathbf{I},$$

(a) Ra = 20,000



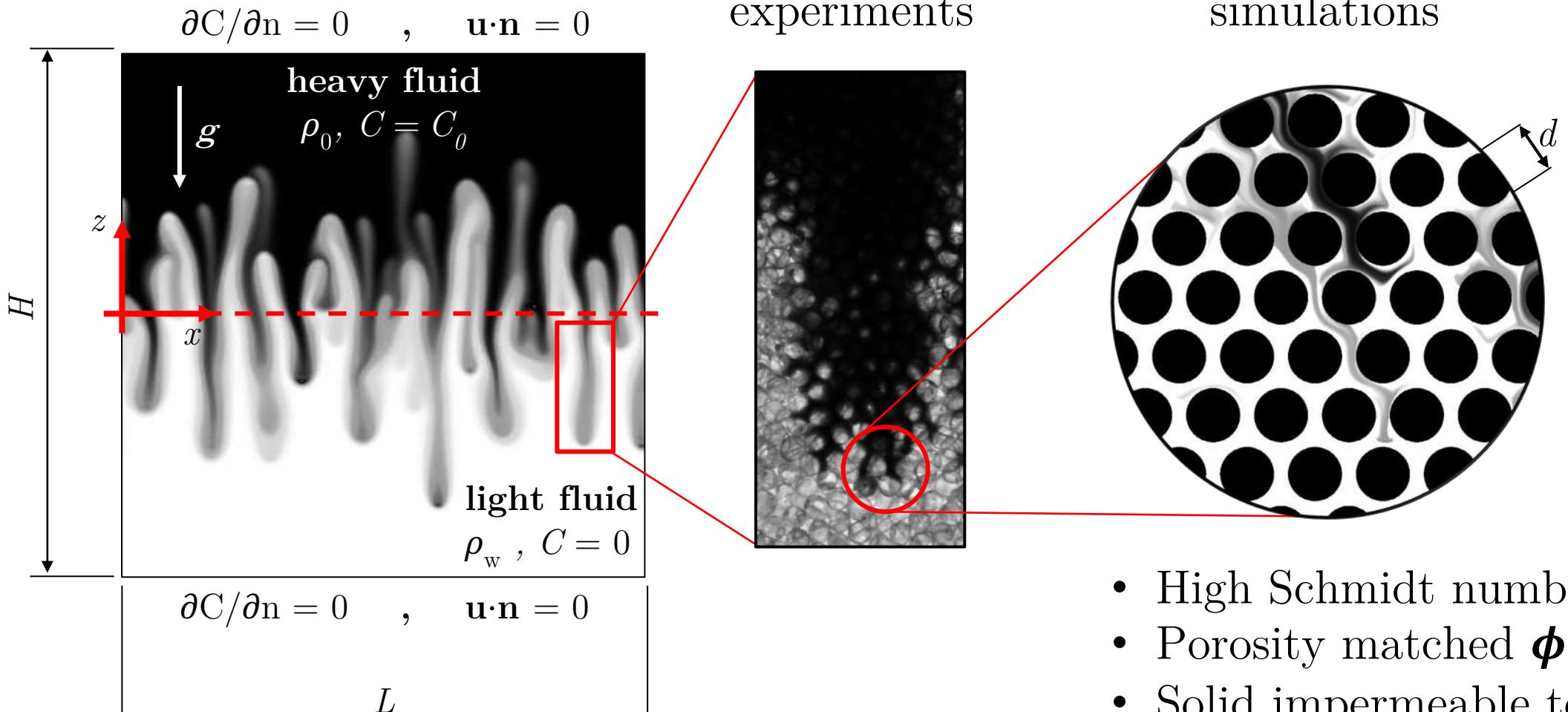
(b) Ra = 20,000



Liang et al., *Geophys. Res. Lett.* (2018)
Chang et al., *Phys. Rev. Fluids* (2018)

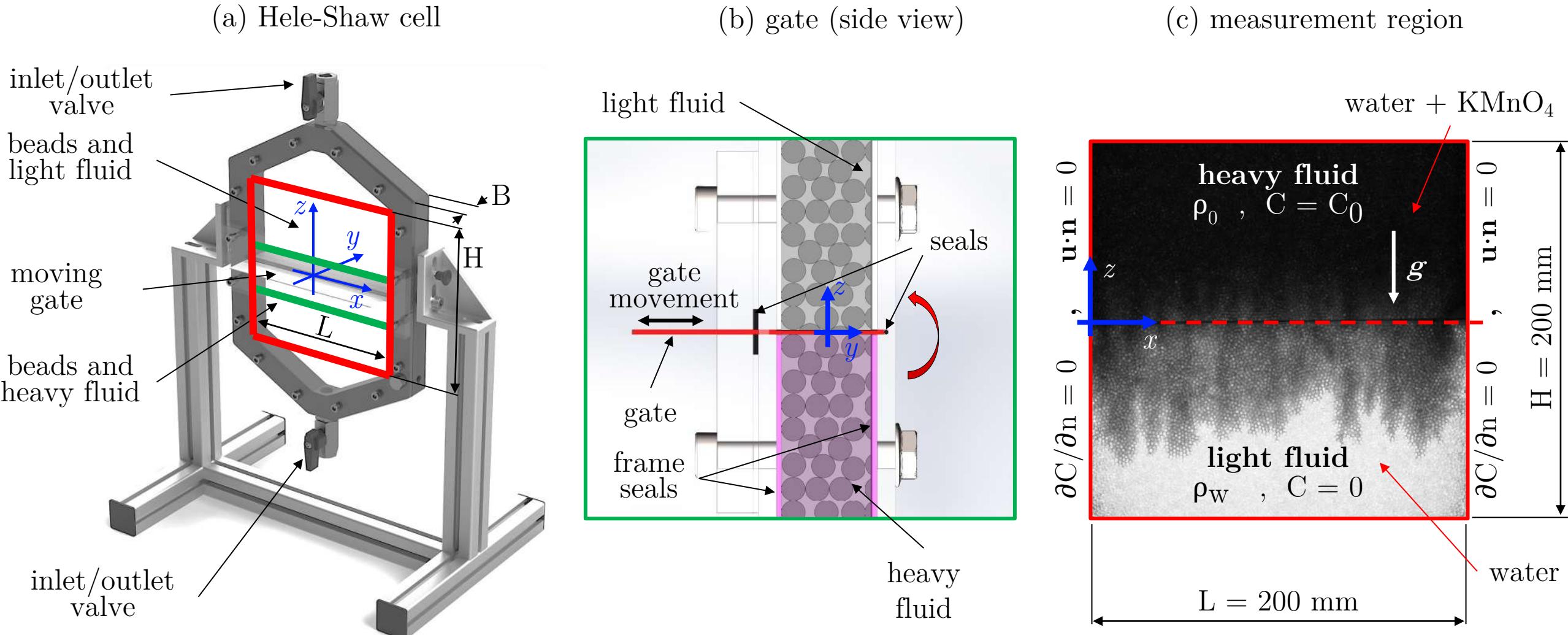
**These models required validation:
Experiments and simulations in porous media**

Flow configuration

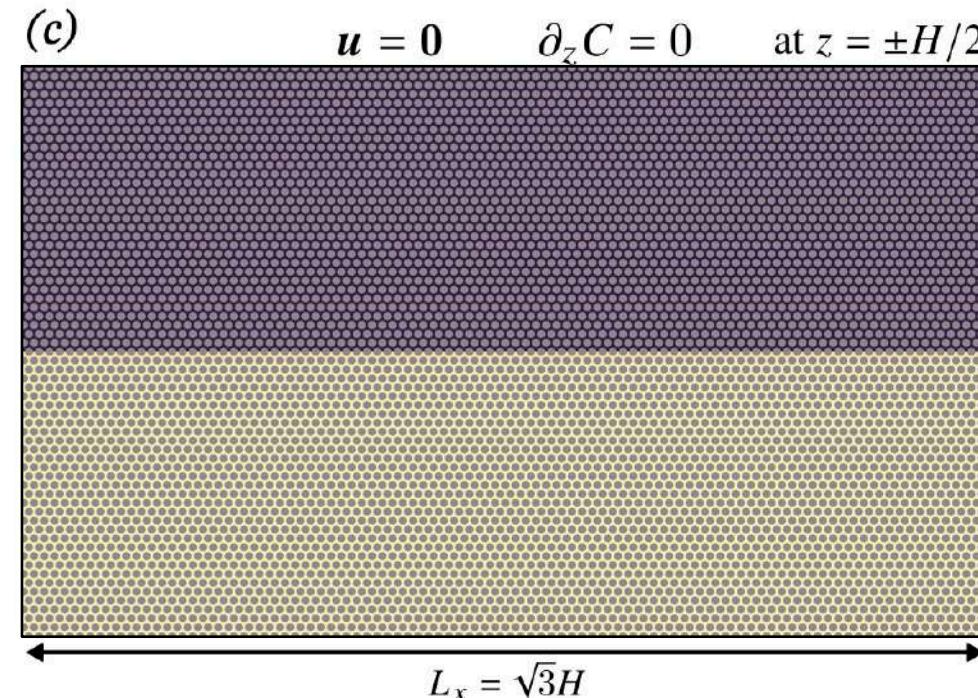
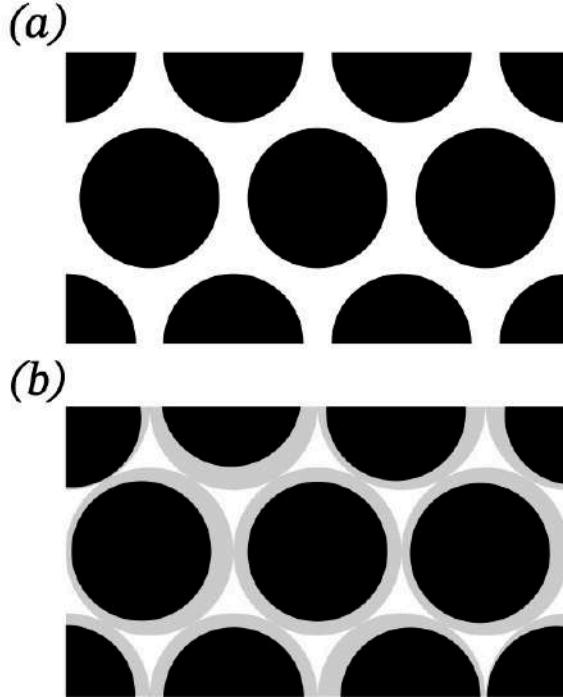


- High Schmidt number
- Porosity matched $\phi = 0.37$
- Solid impermeable to solute
- Linear dependency $\rho(C)$

Experimental setup



Numerical method



$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\rho_0^{-1} \nabla p + \nu \nabla^2 \mathbf{u} - g \beta C \hat{\mathbf{z}},$$

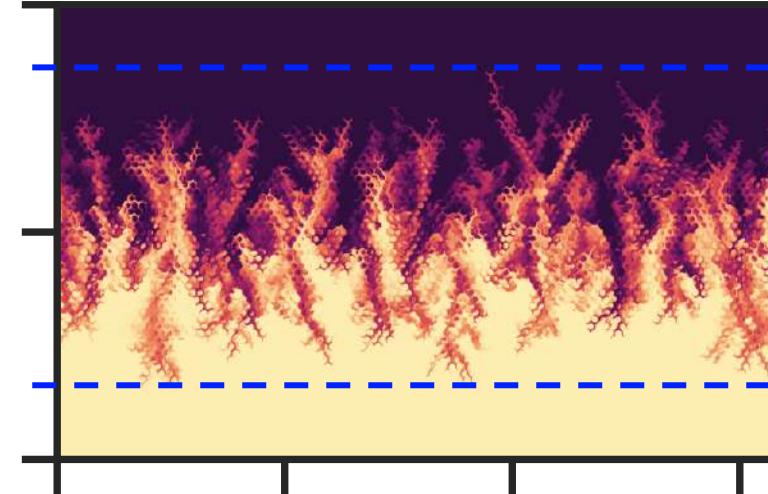
$$\partial_t C + (\mathbf{u} \cdot \nabla) C = D \nabla^2 C,$$

$$\rho = \rho_0 \left[1 + \frac{\Delta \rho}{\rho_0 C_0} (C - C_0) \right]$$

Finite difference
(AFID, open
source)
+
Immersed
Boundaries Method

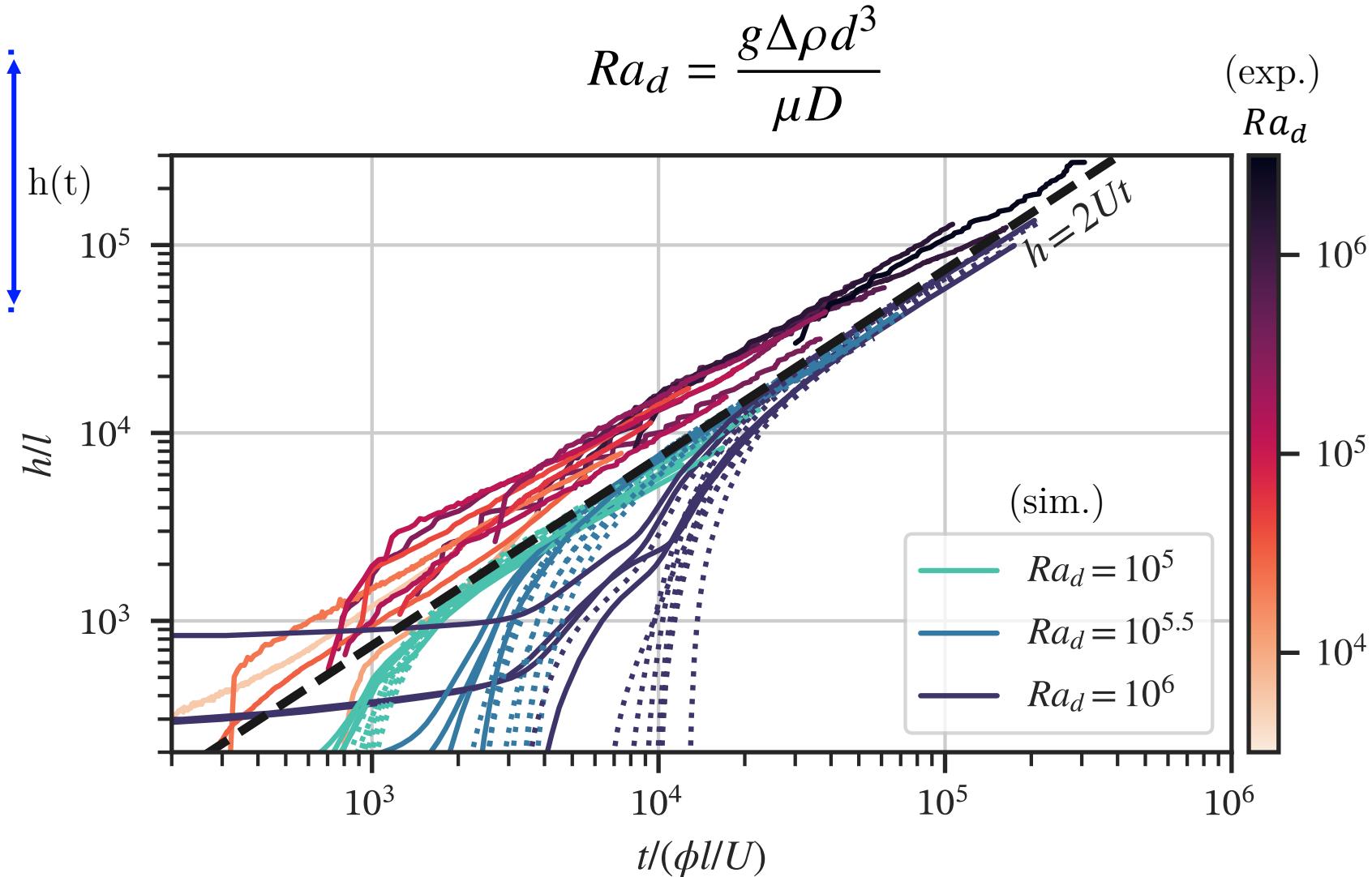
- Resolution:
- velocity: ≥ 32 points per diameter
 - conc. : ≥ 128 points per diameter

Mixing length



$$U = \frac{g\Delta\rho k}{\mu}$$

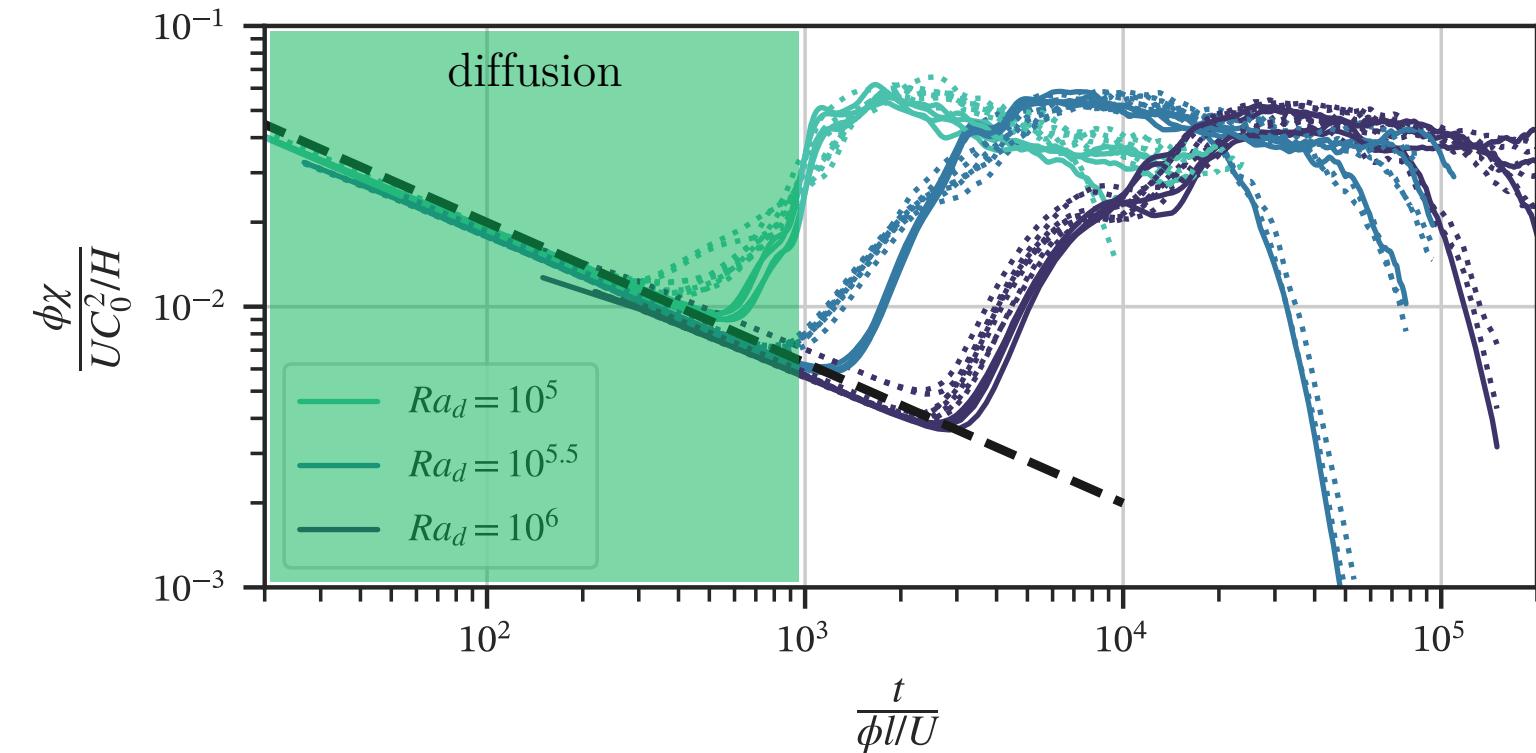
$$\ell = \frac{\phi D}{U}$$



Modelling scalar dissipation

$$\chi = D \langle |\nabla C|^2 \rangle_f = \frac{D}{V_f} \int_{V_f} |\nabla C|^2 \, dV$$

Can we model this mixing/dissolution process?



Diffusion:

$$C = C_0 + \frac{\Delta C}{2} \operatorname{erf} \left(\frac{z}{\sqrt{2\kappa t}} \right)$$

$$\partial_z C = \frac{\Delta C}{2\sqrt{\pi\kappa t}} \exp \left(-\frac{z^2}{2\kappa t} \right)$$

$$\begin{aligned} \chi &= \kappa \langle |\nabla C|^2 \rangle = \frac{\kappa}{H} \int_{-\infty}^{\infty} |\partial_z C|^2 dz \\ &= \sqrt{\frac{\kappa}{8\pi t}} \frac{(\Delta C)^2}{H} \end{aligned}$$

Modelling scalar dissipation

$$\chi = D \langle |\nabla C|^2 \rangle_f = \frac{D}{V_f} \int_{V_f} |\nabla C|^2 \, dV$$

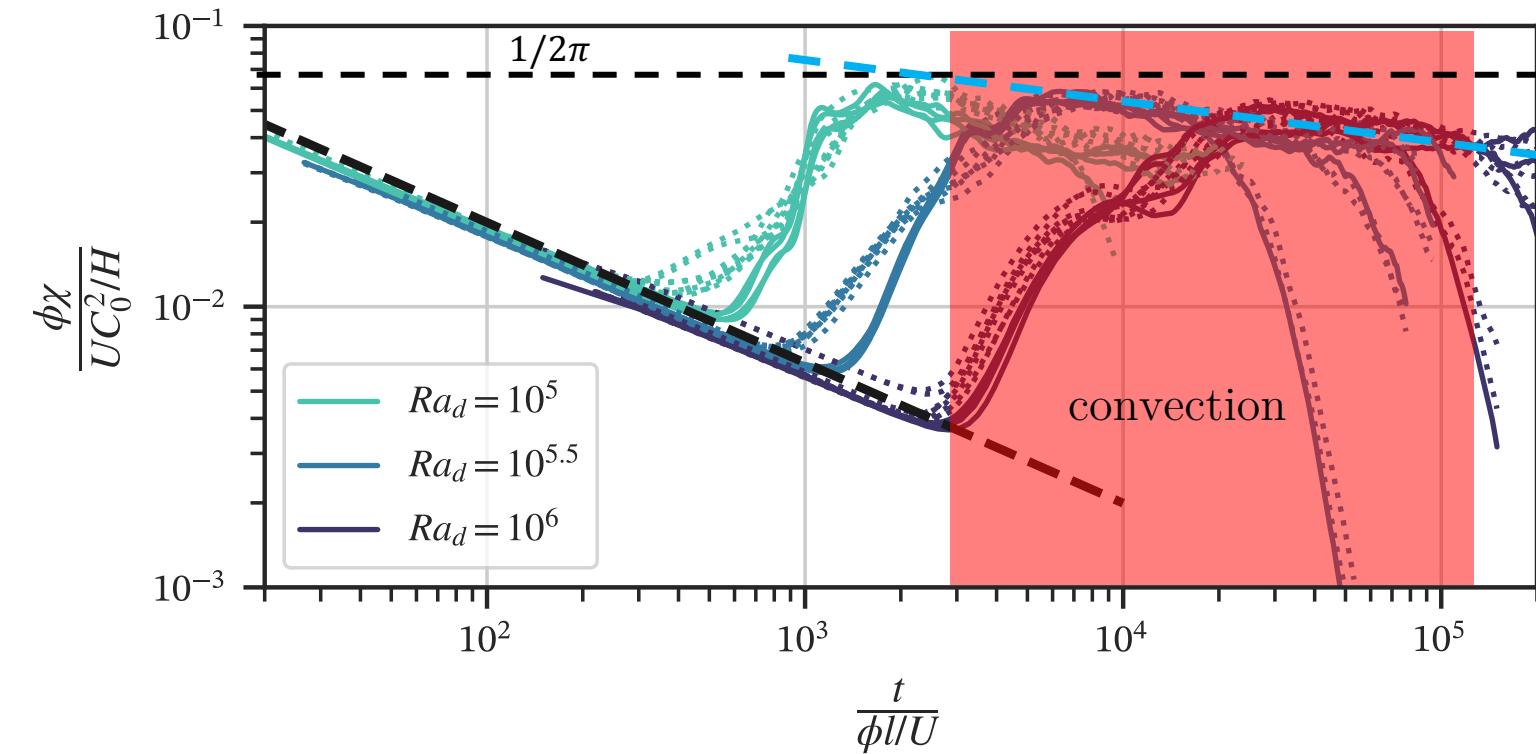
Convection

$$\chi = \kappa \langle |\nabla C|^2 \rangle = \kappa \frac{L_m}{H} \langle |\nabla C|^2 \rangle_{ML},$$

$$|\nabla C| \approx \frac{\Delta C}{2\sqrt{\pi\kappa t}}.$$

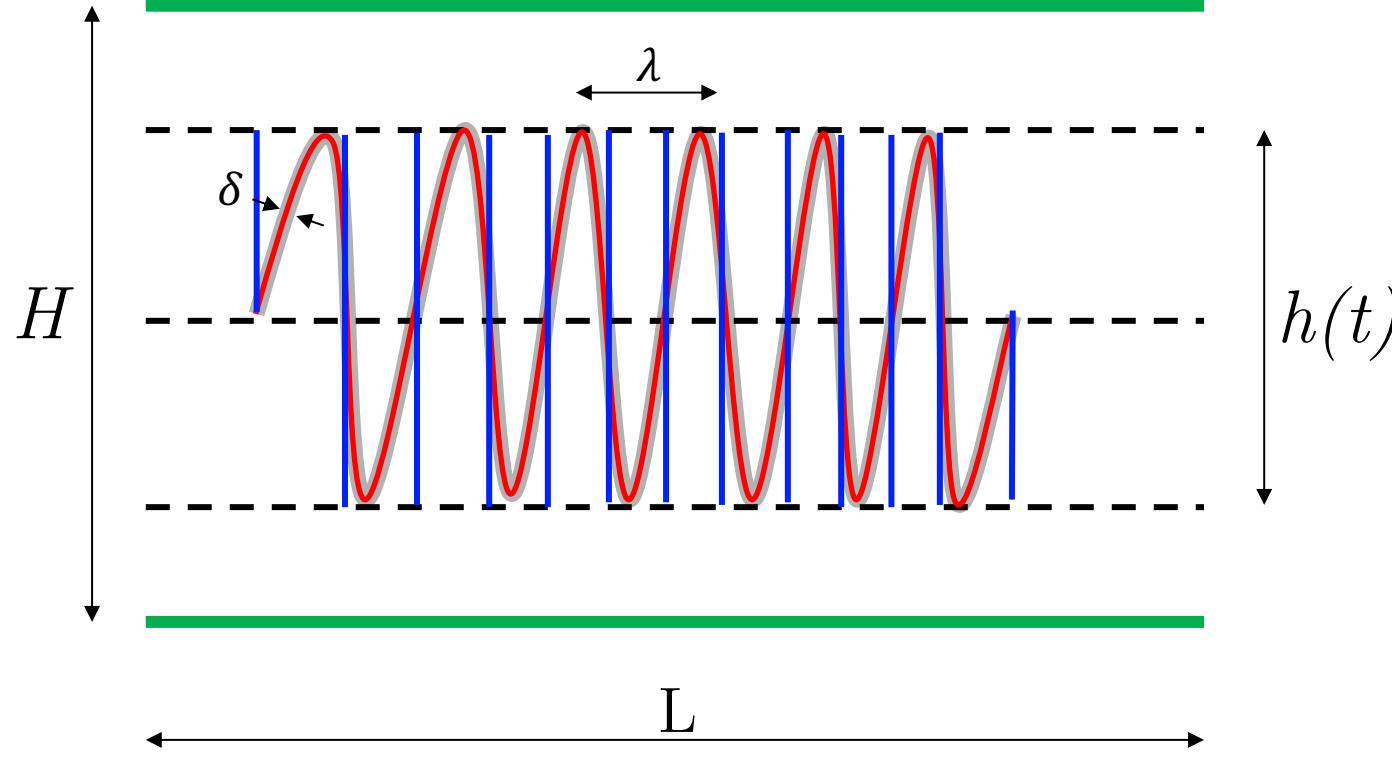
$$L_m \approx 2Ut,$$

$$\chi \approx \kappa \frac{2Ut}{H} \frac{(\Delta C)^2}{4\pi\kappa t} = \frac{1}{2\pi} \frac{U_d(\Delta C)^2}{H}.$$

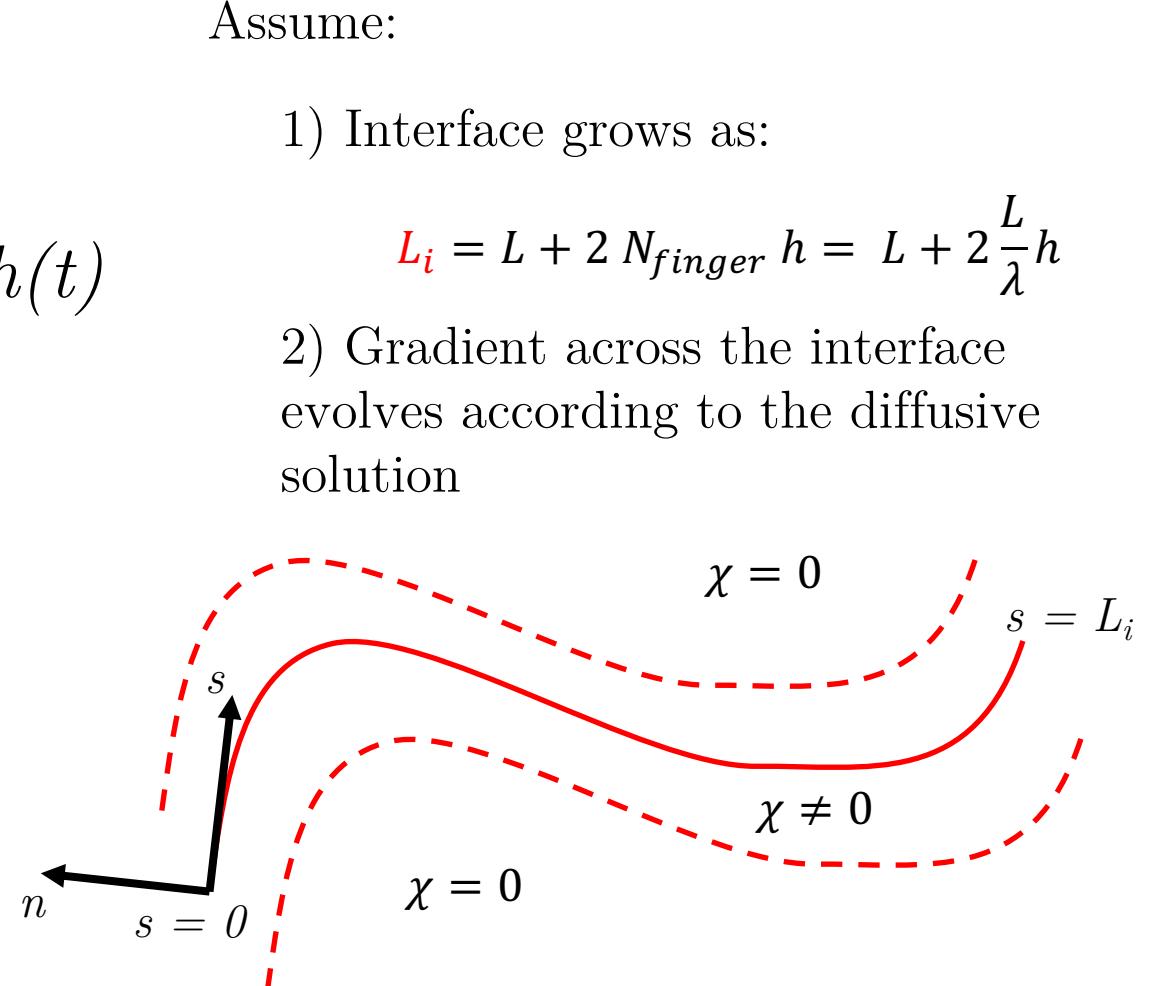


$1/2\pi$ is the maximum value of dissipation. Practically, χ decreases with time

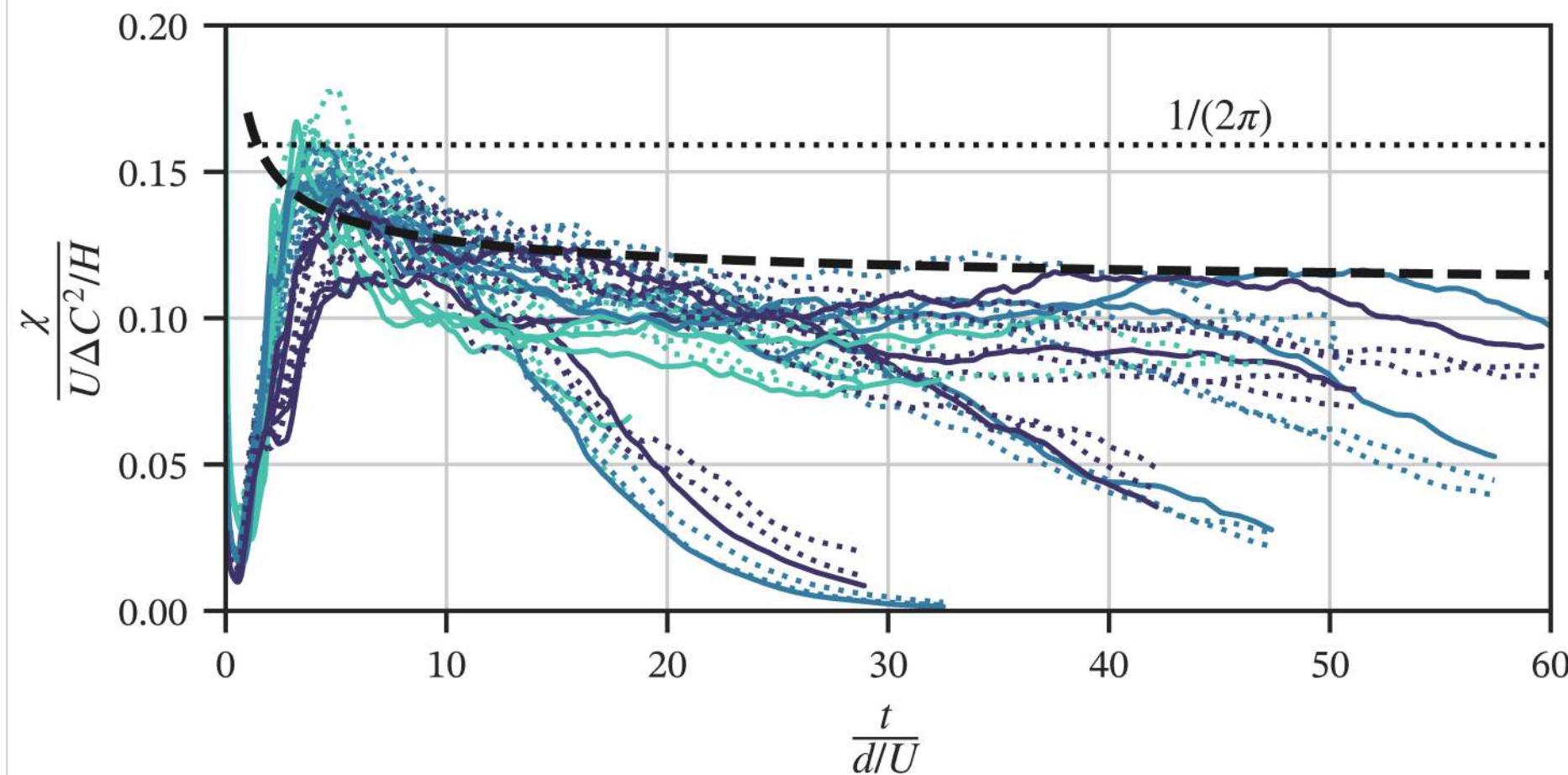
Modelling scalar dissipation



$$\chi = D \langle |\nabla C|^2 \rangle = \frac{D L_i}{H L} \int_{-\delta/2}^{+\delta/2} |\partial_n C|^2 dn$$



Modelling scalar dissipation

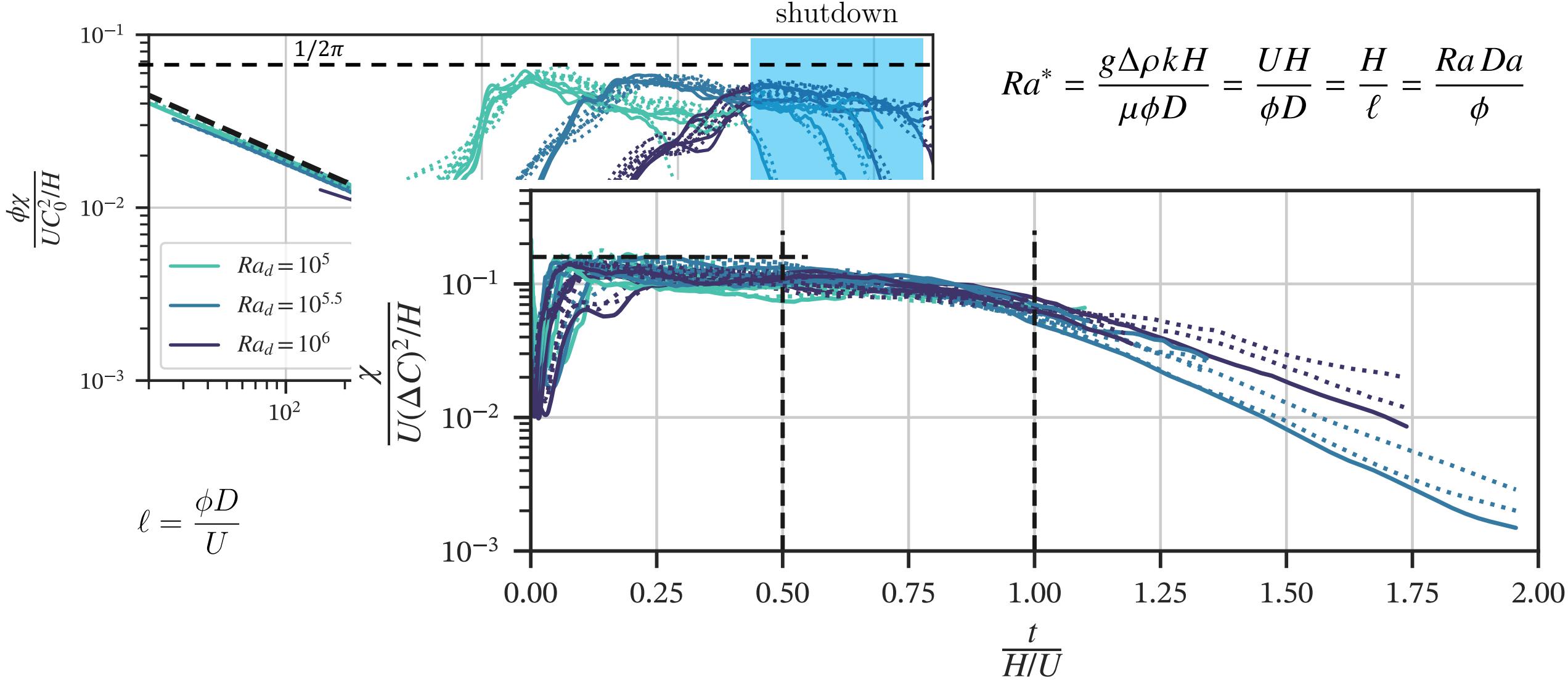


$1/(2\pi)$ is the maximum value of dissipation.

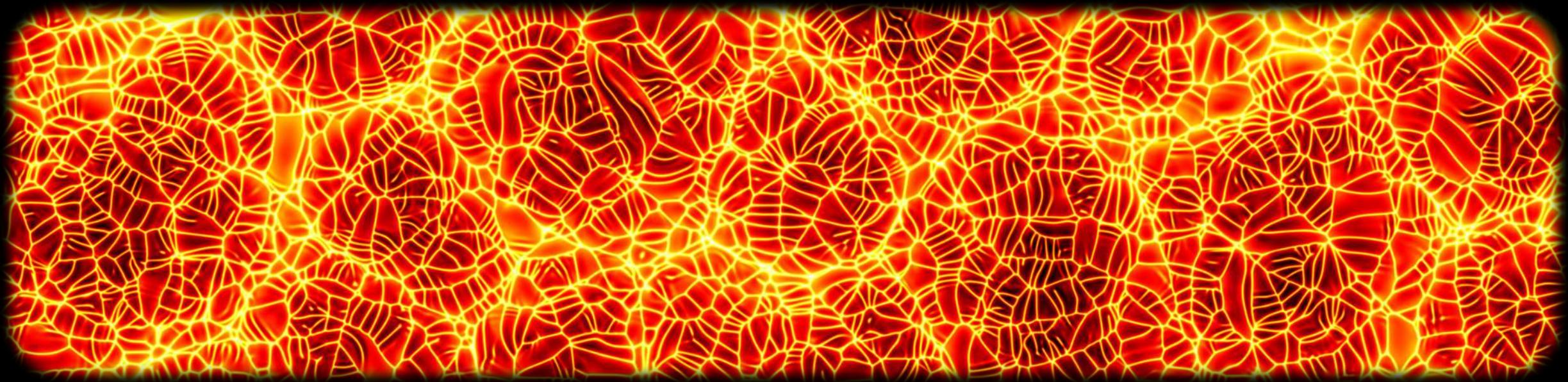
Model shown starting from $t/(d/U) = 1$.
Time is also increased by d/U to account for initial condition.

$$\frac{\chi(t=1)}{(\Delta C)^2 U / H} = \frac{\beta}{\alpha \pi} \left(1 + \frac{\alpha}{4}\right) \approx \frac{1}{1.92\pi} \approx \frac{1}{2\pi}$$

Modelling scalar dissipation

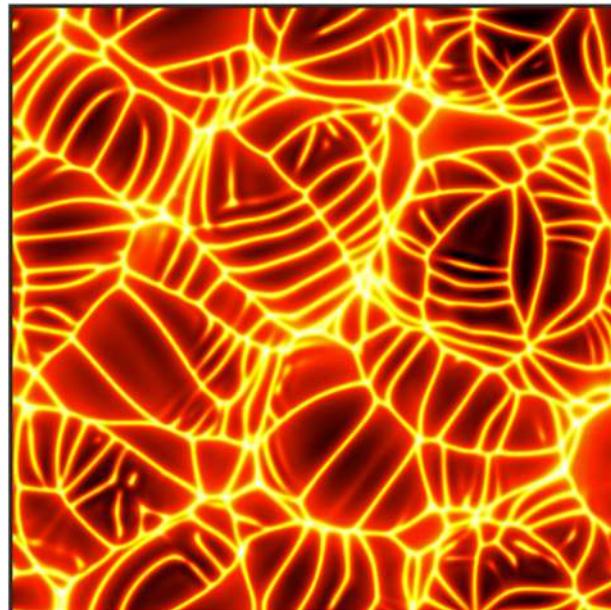
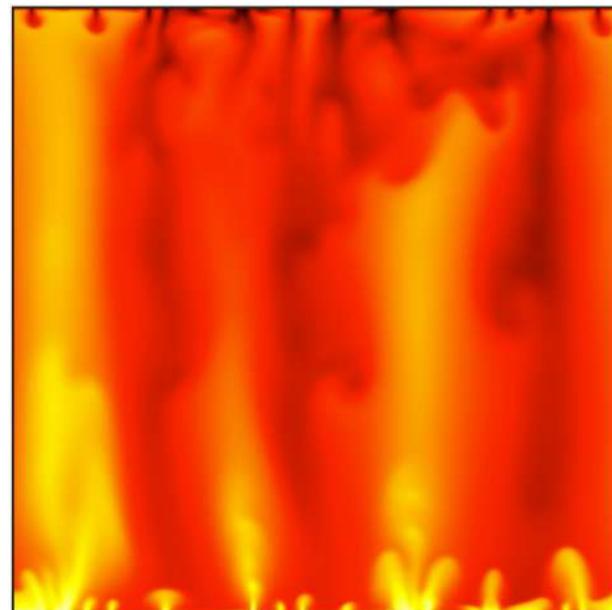


1. Motivation
2. Reservoir-scale: multiphase gravity currents
3. Darcy-scale: simulations, experiments and finite-size effects
4. Pore-scale modelling and dispersion
5. Conclusions and outlook



Conclusions and outlook

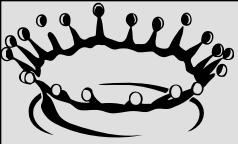
1. Convection in porous media is a **multiscale** and **multiphase** process
2. A **combination of experiments, simulations and theory** is required to model the flow dynamics
3. Recent developments in numerical and experimental capabilities enable measurements at unprecedented level of detail, but the parameters space is huge!



pore-scale



<https://arxiv.org/abs/2310.04068>



Physics of Fluids

Conclusions and outlook

Thank you for your
attention! Questions?

Physics Today 74, 5, 68 (2021)

High-resolution images, movies and slides are available upon request to m.depaoli@utwente.nl