Lab. of Complex Fluids
and its Reservoirs

Solute dispersion in confined porous media: Insights from experiments, simulations, and modelling

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Physics of Fluids

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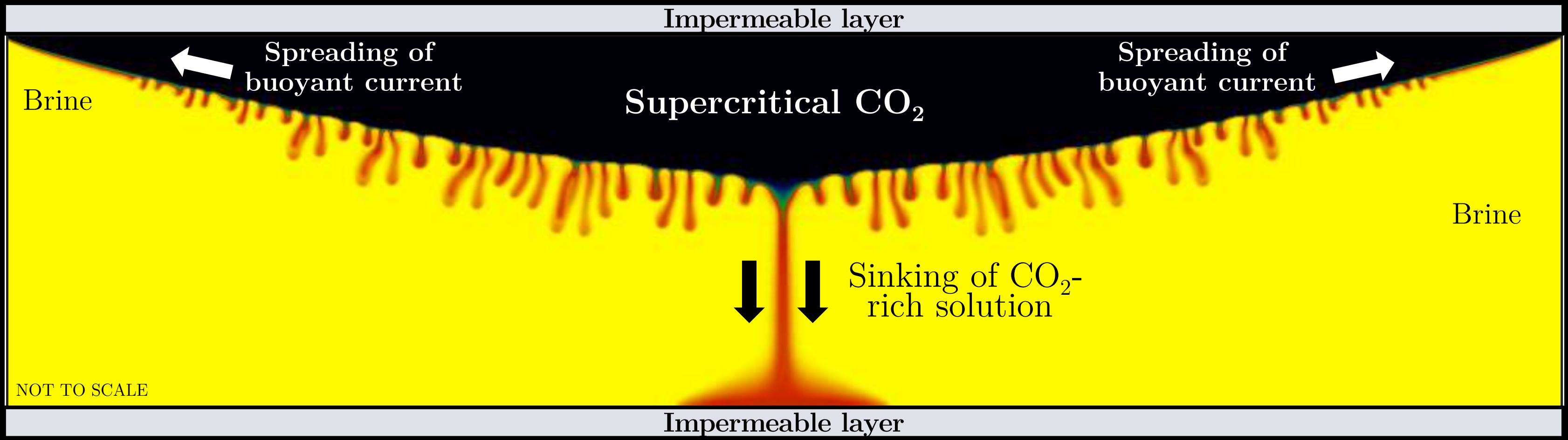
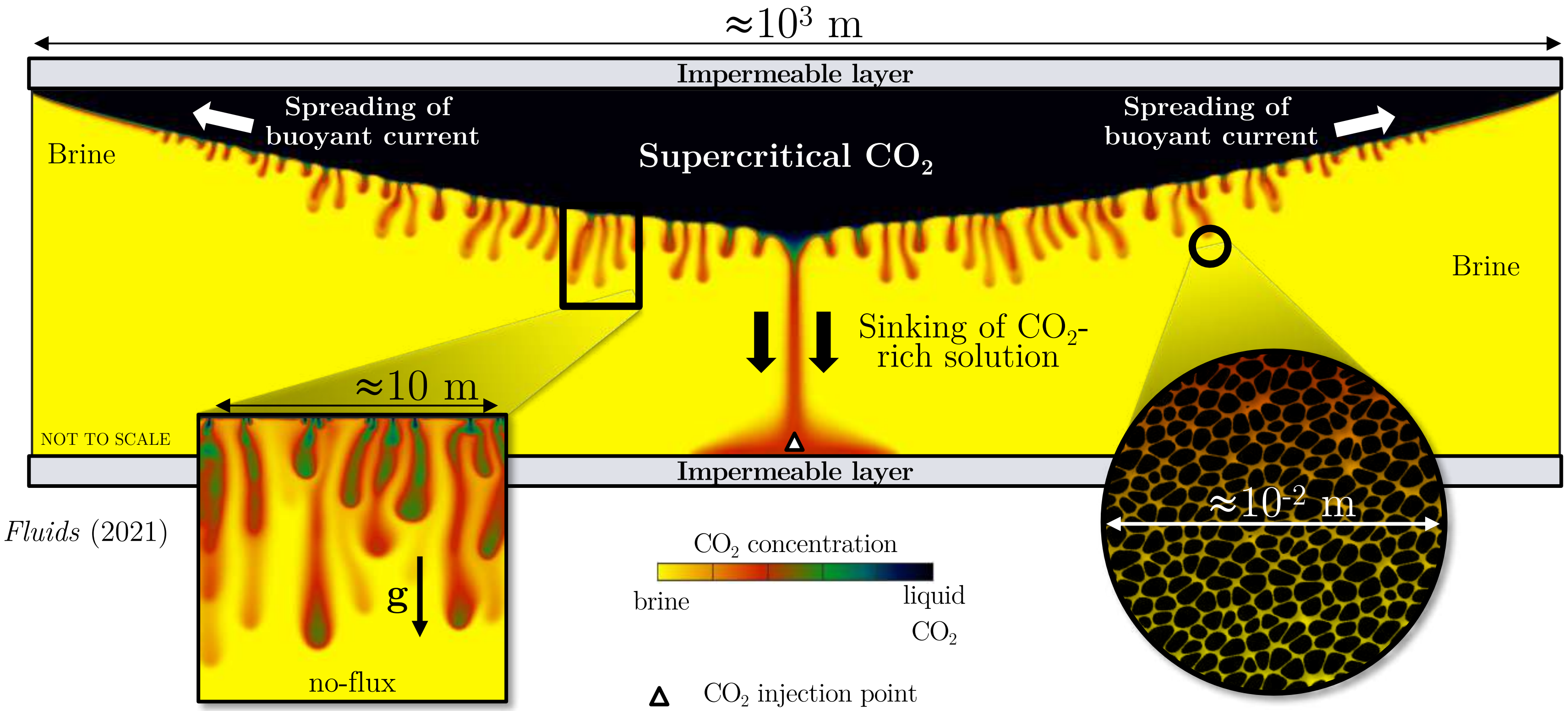
Presentation outline

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

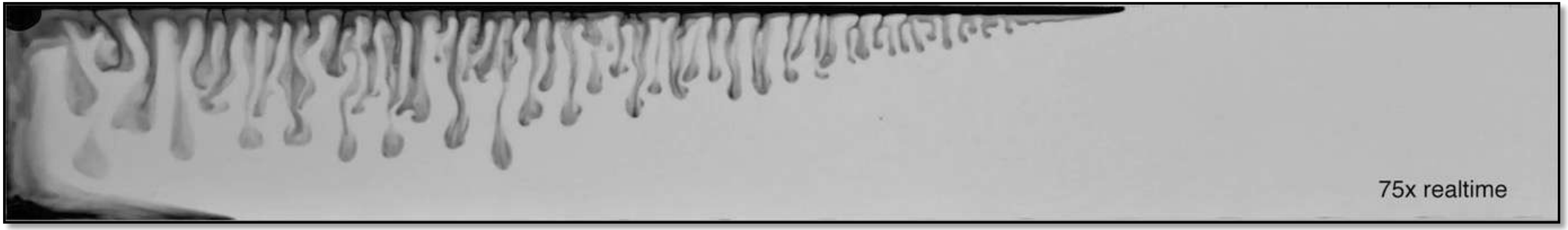


Carbon Capture and Storage



De Paoli, *Phys. Fluids* (2021)

MacMinn et al., *Geophys. Res. Lett.* (2013)



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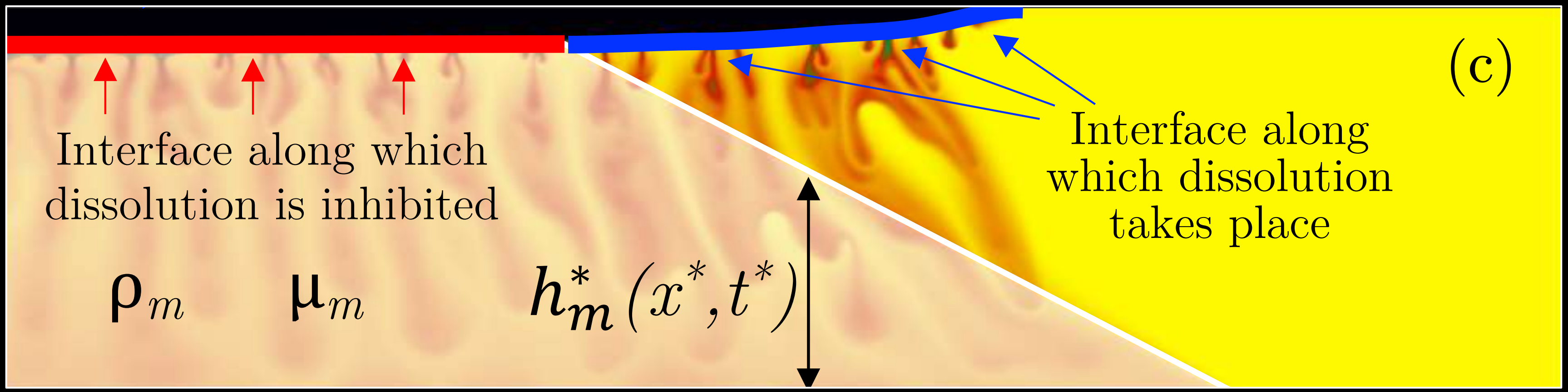

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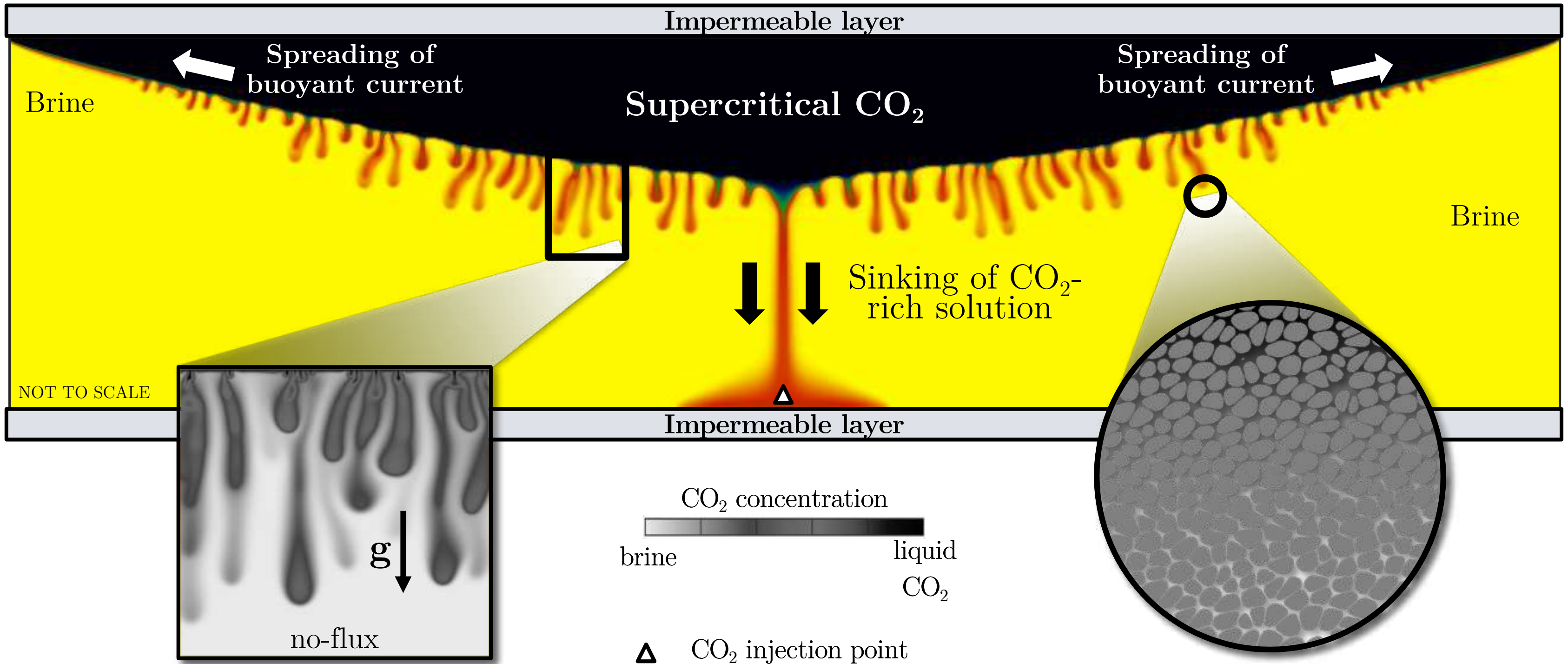
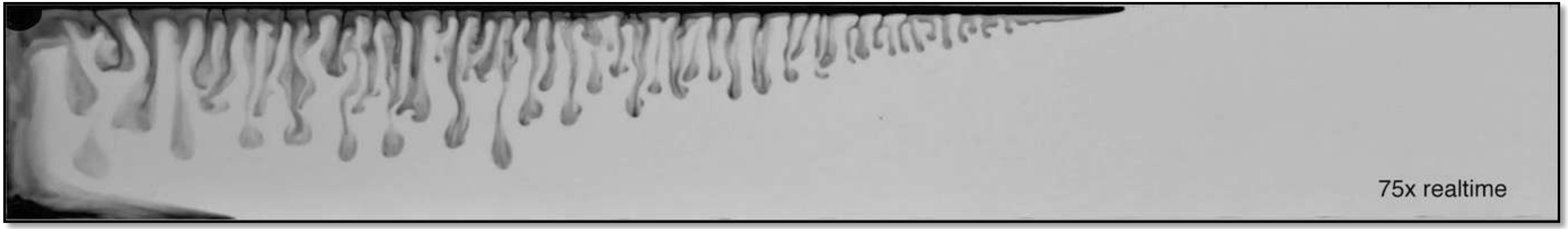


De Paoli, *Phys. Fluids* (2021)

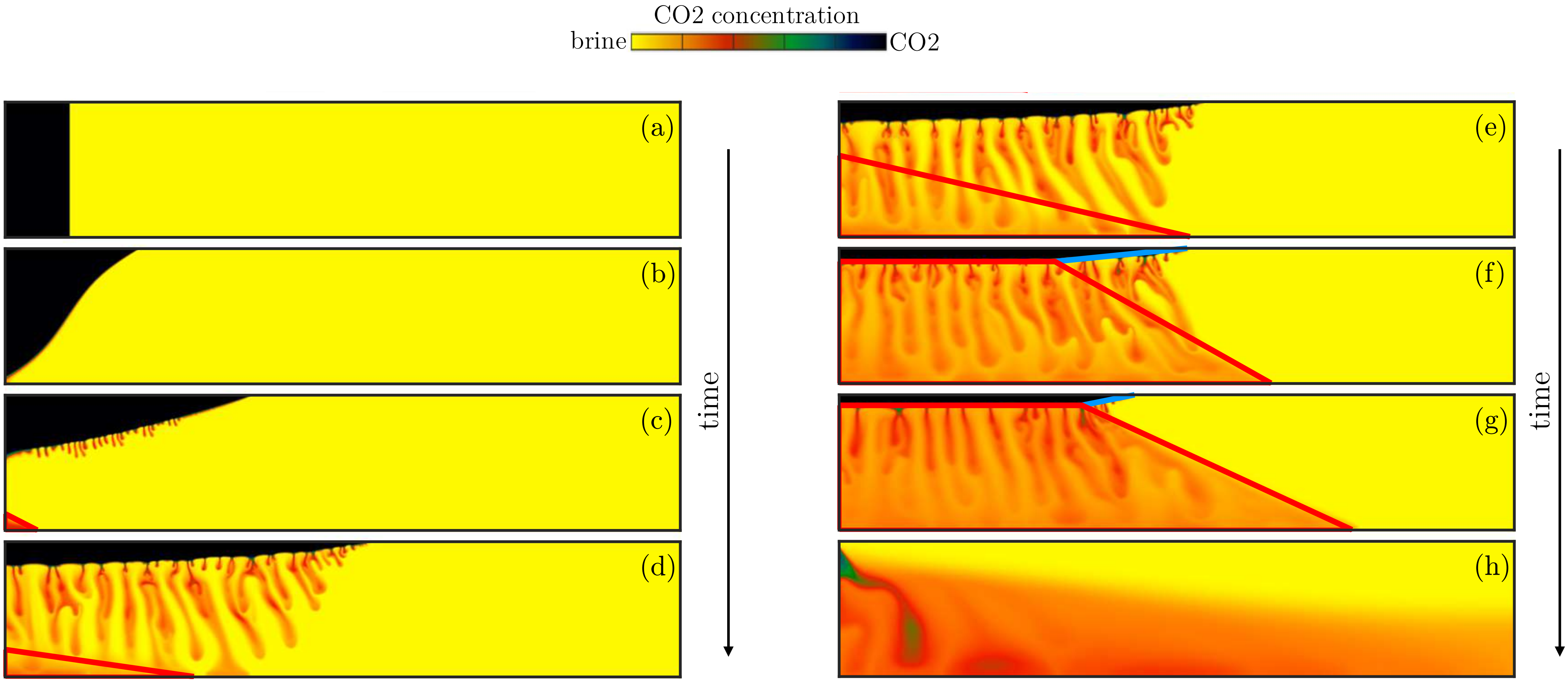
Reservoir properties

- 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)

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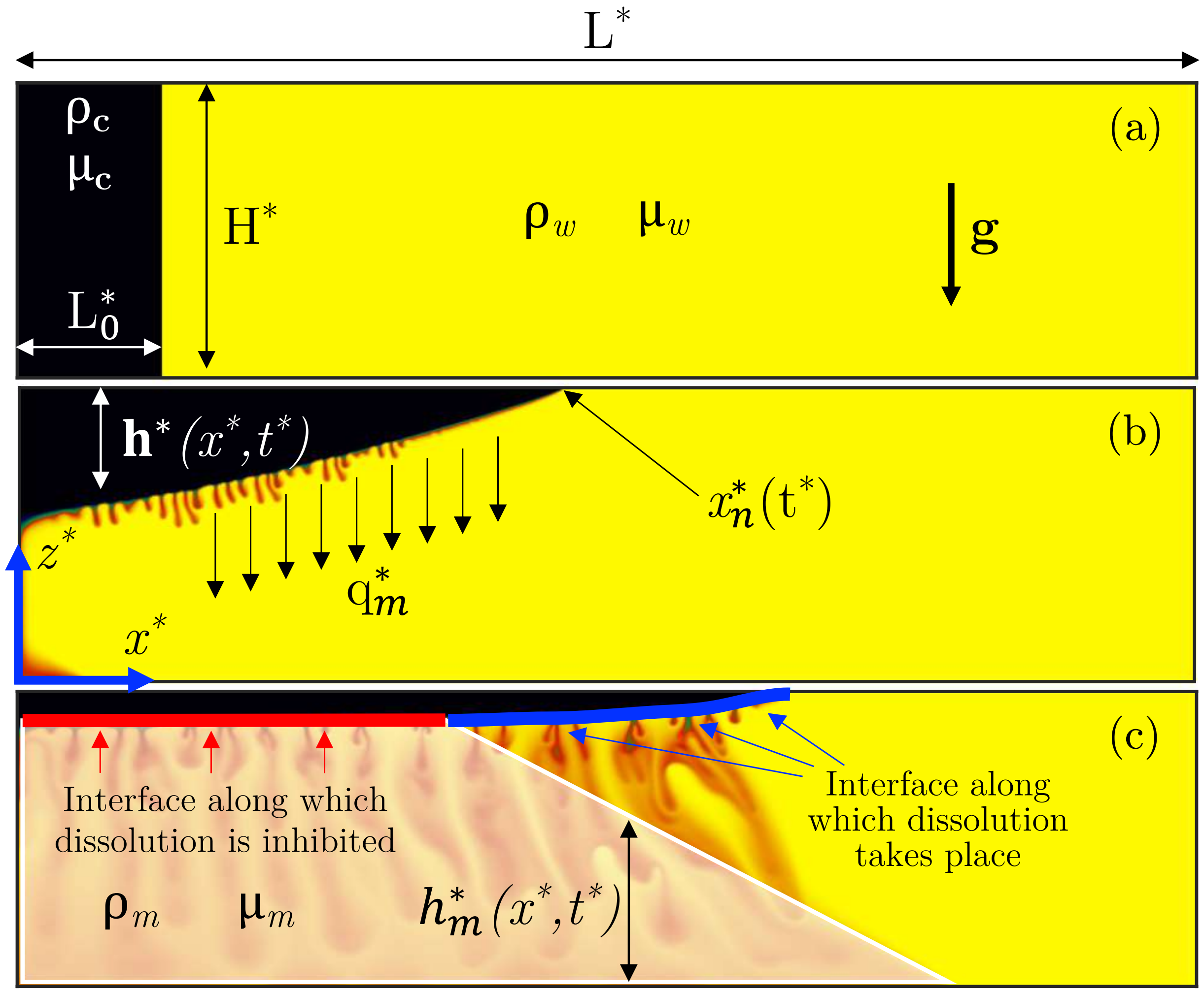
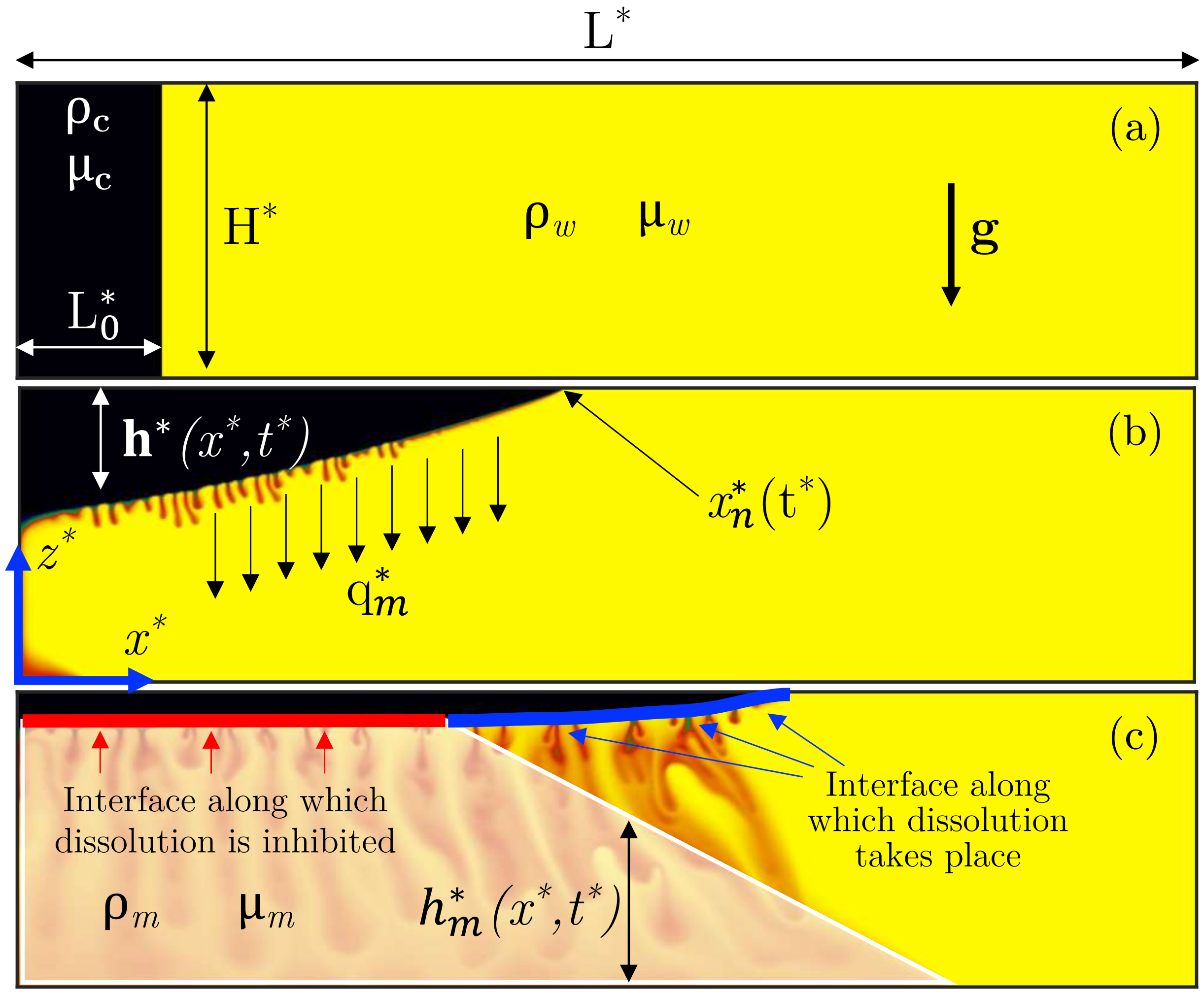


De Paoli, *Phys. Fluids.* (2021)

$$\nabla \cdot \mathbf{u_i}^* = 0$$

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

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



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

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

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

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

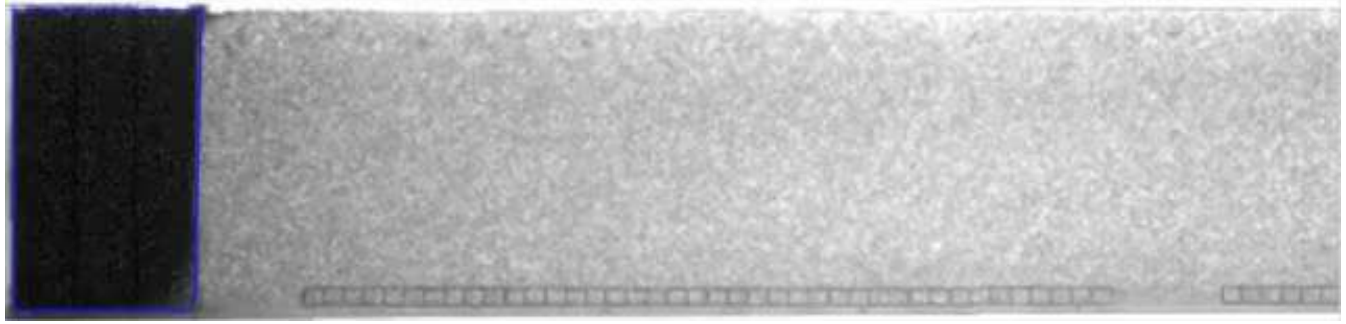
$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

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

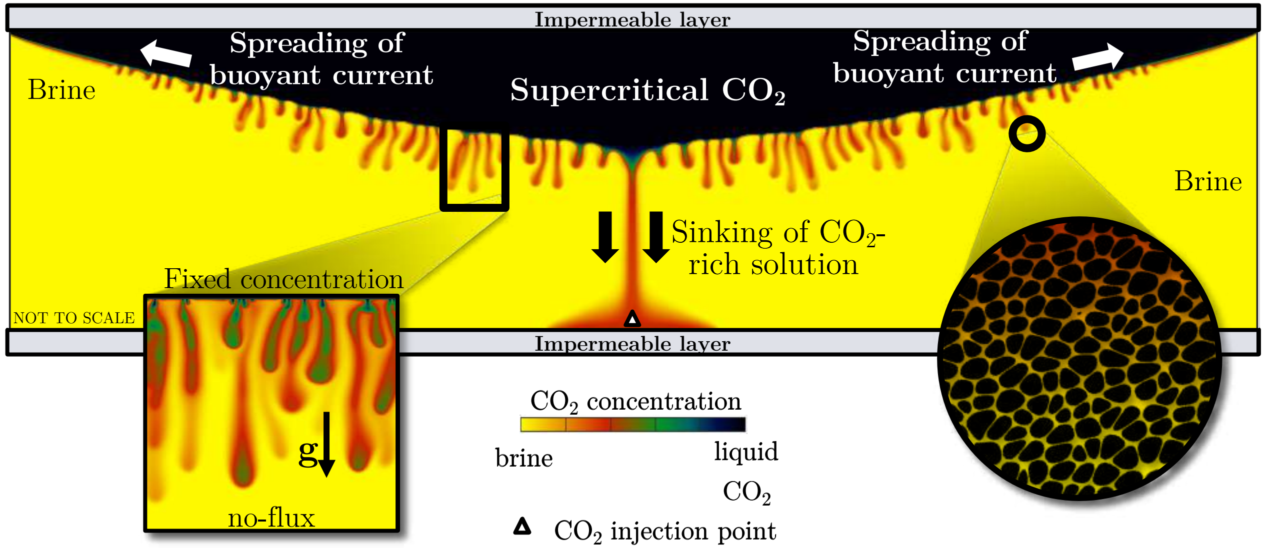
Mobility ratios $M = \mu_w/\mu_c$ and $M_m = \mu_w/\mu_m$

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

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



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



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

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

How to determine the dissolution rate q_m^* ?

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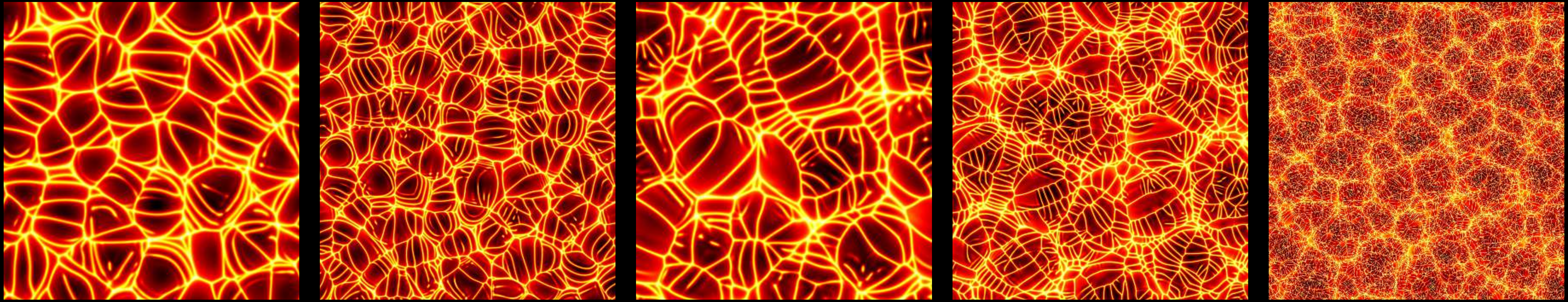


Darcy numerical simulations

Dimensionless equations

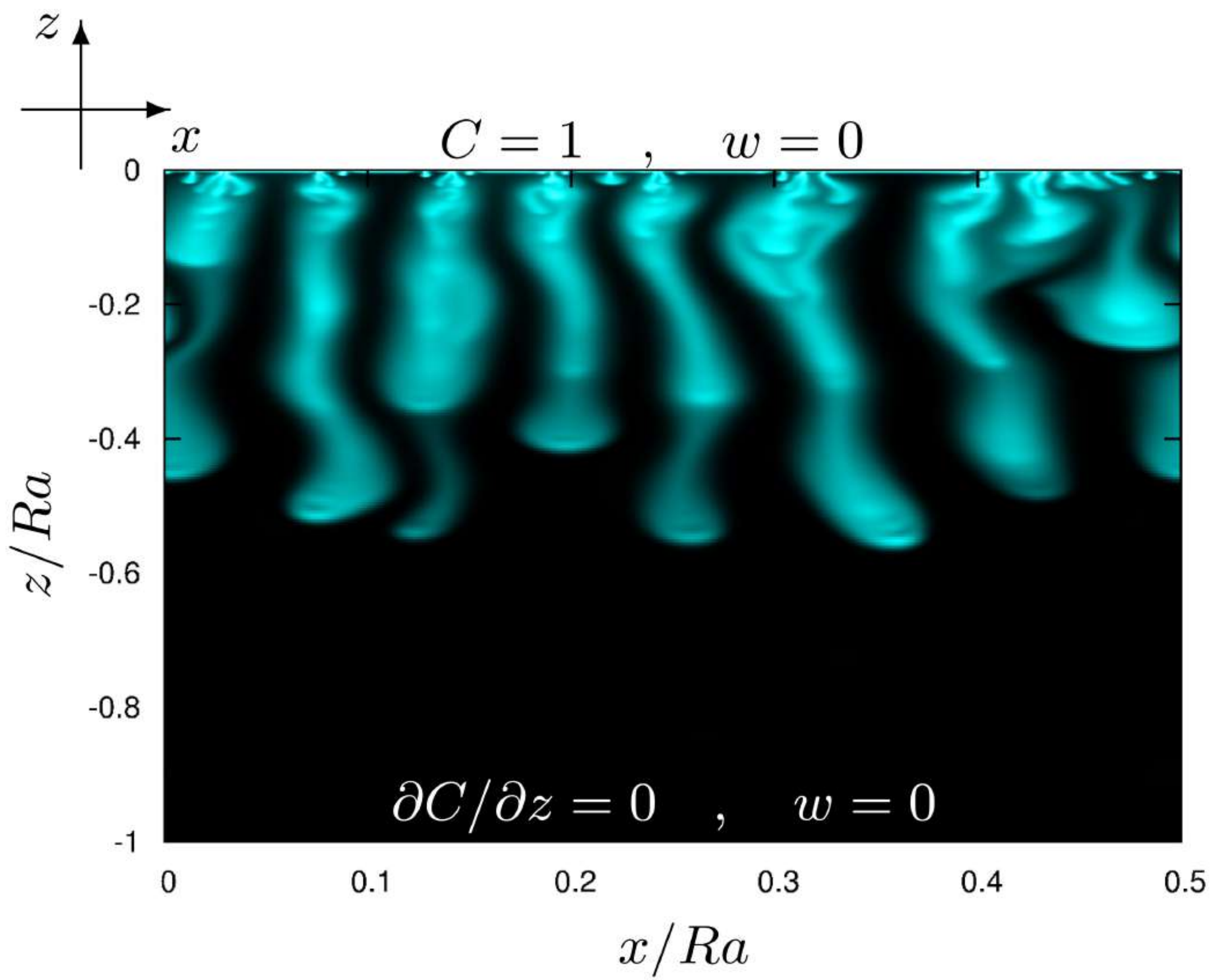
$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} = \frac{1}{Ra}\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

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

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

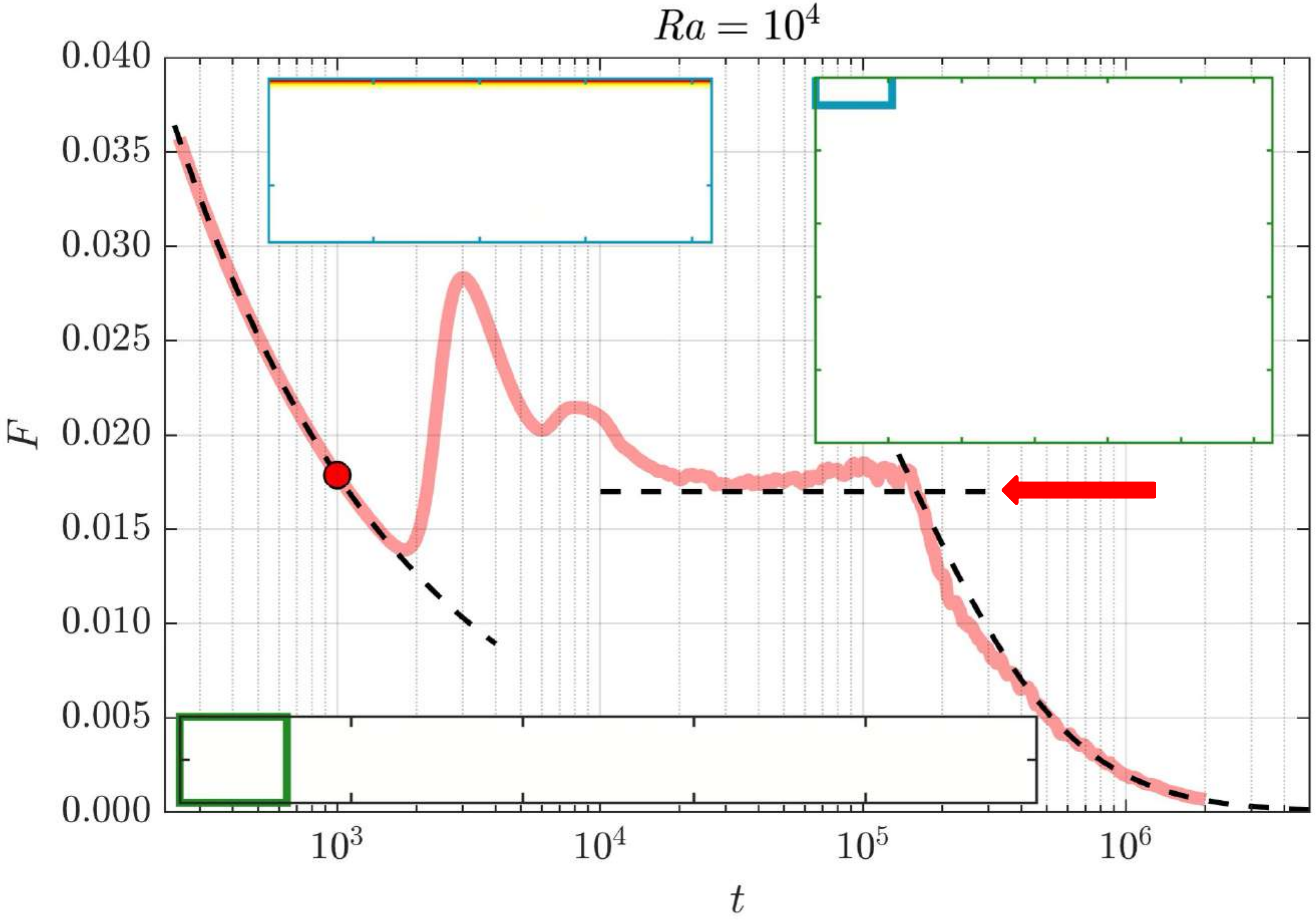
Governing parameter

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



Convective dissolution process

$$F(t) = \frac{1}{L}\int_0^L \frac{\partial C}{\partial z}\bigg|_{z=0} dx$$



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

Convection in anisotropic media

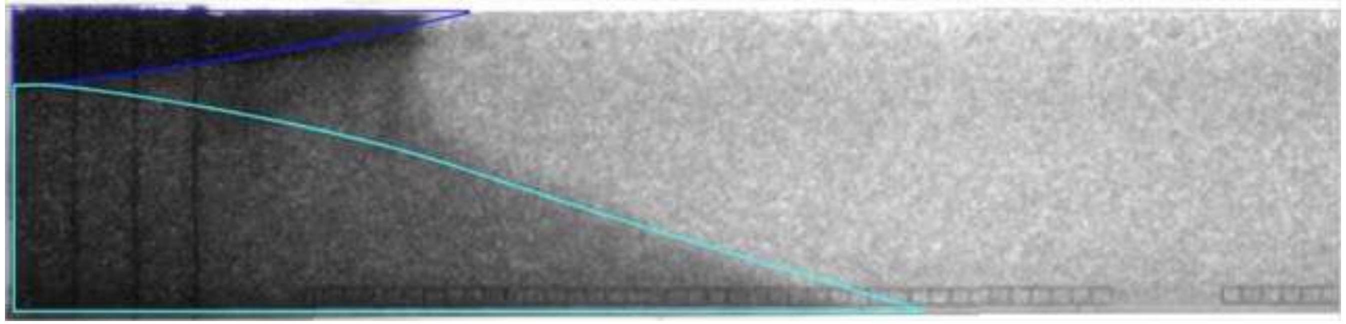
Examples of model extension:
effect of **anisotropy** of the medium

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

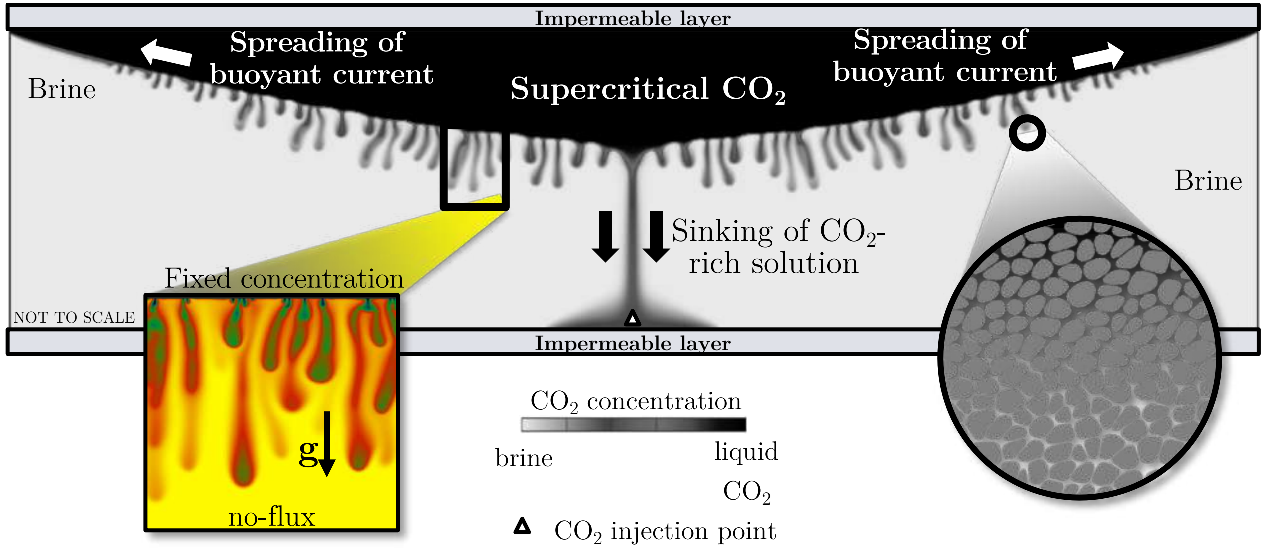
Sedimentary rocks: Rocks formed by stratification

benedek / Getty Images

Rhododendrites/Wikimedia Commons/CC BY 4.0



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



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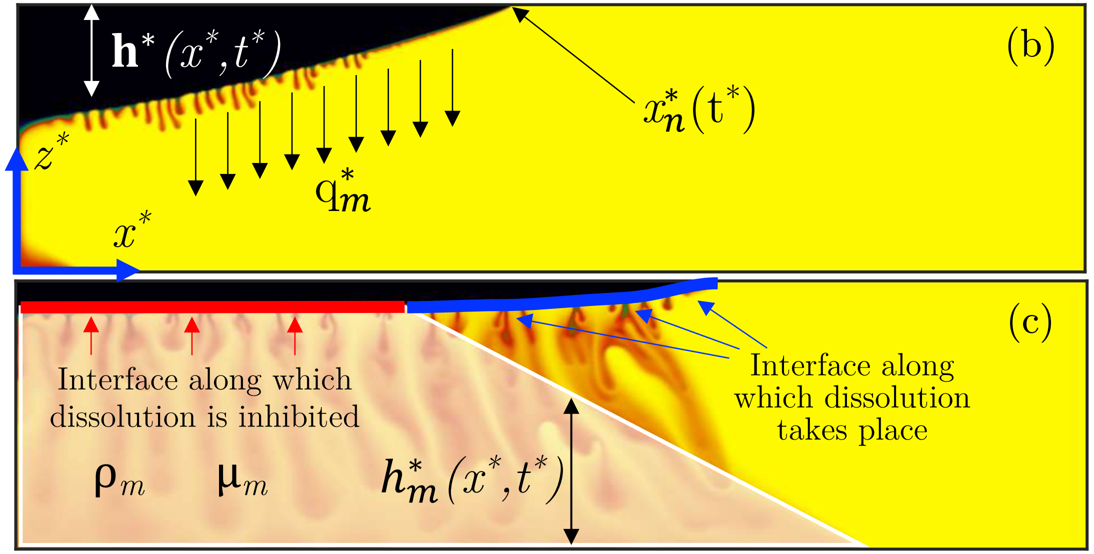
How to determine the dissolution rate q_m^* ?

Effect of anisotropy



Darcy-scale simulations:

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

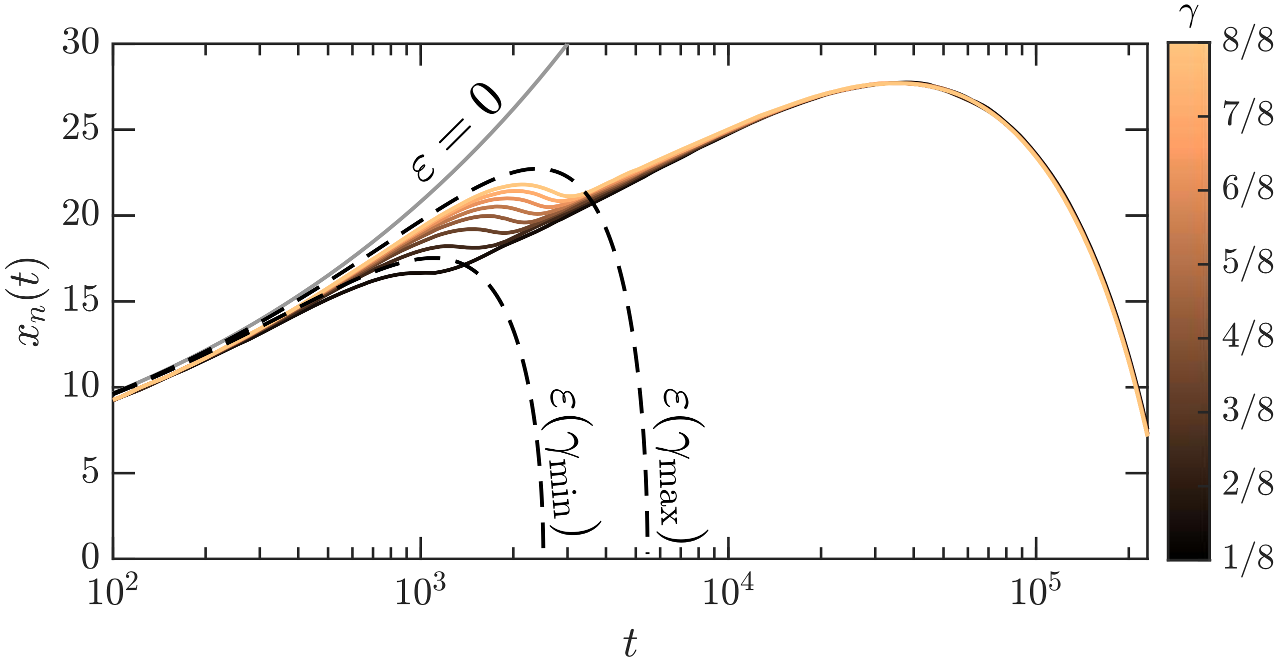
dissolution increases with the anisotropy of the medium

Sedimentary rocks are anisotropic

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

$\gamma = 1$ isotropic

$\gamma = 1/8$ strongly anisotropic

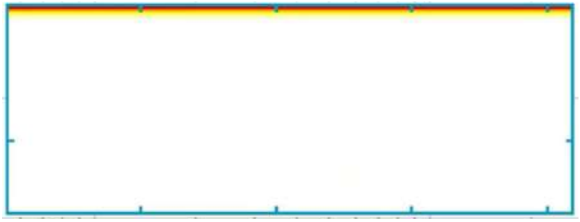


Analytical solution in case of
- no-dissolution
- independent currents

De Paoli, Zonta & Soldati, *Phys. Fluids* (2016, 2017)

Scalings of convection and finite-size effect

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



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

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

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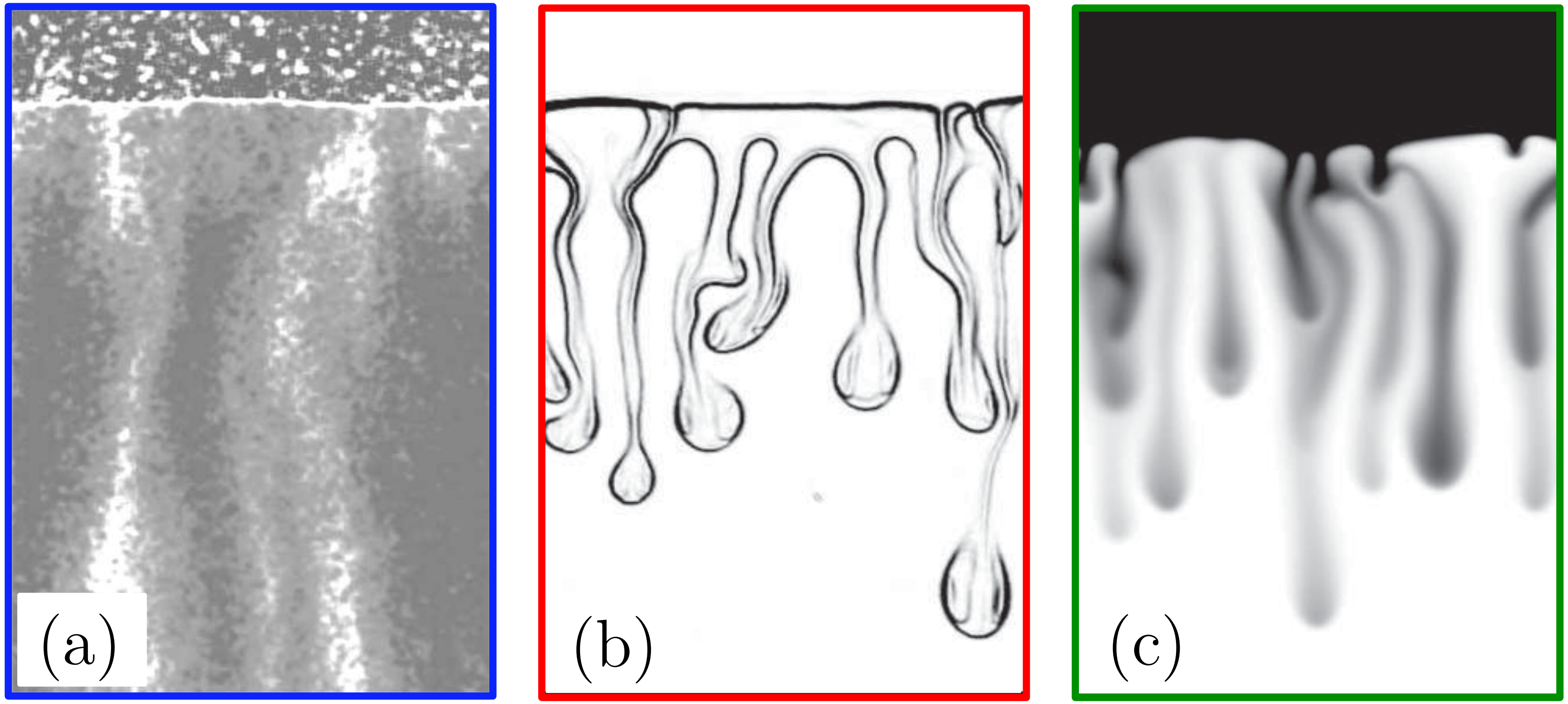

Differences arise due to effects not present in the Darcy model: consequences for **porous media** and **Hele-Shaw**

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

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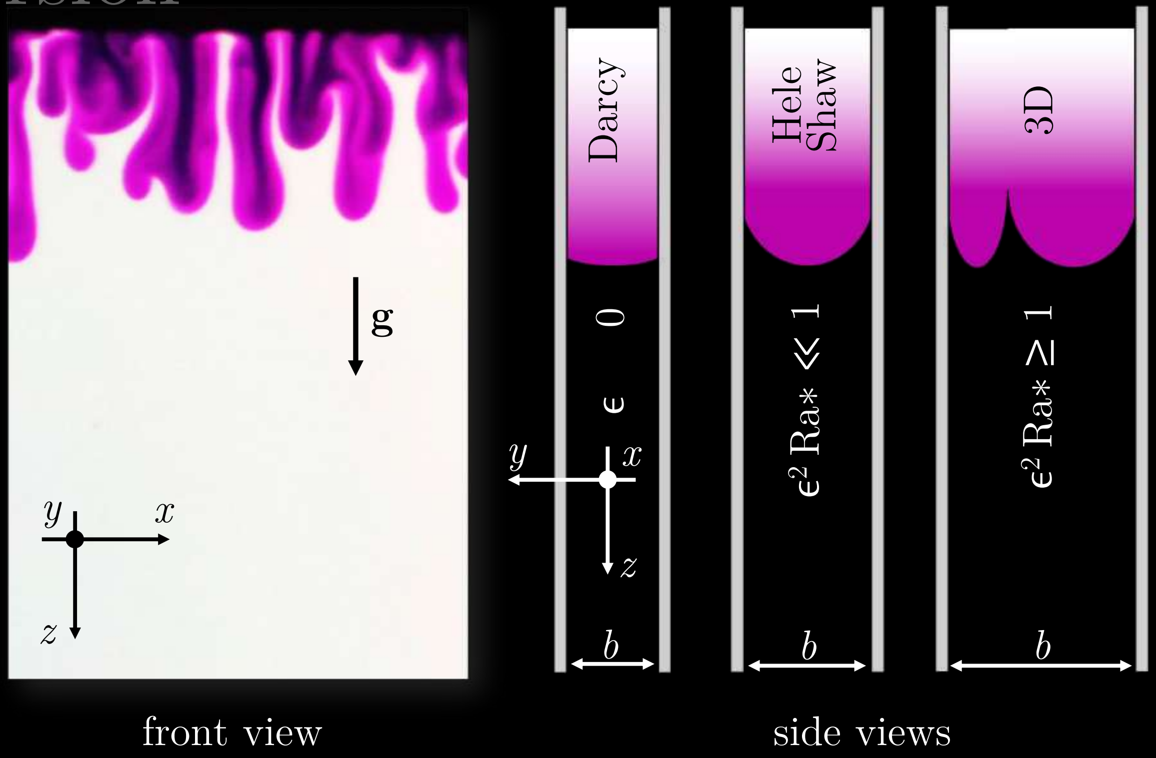

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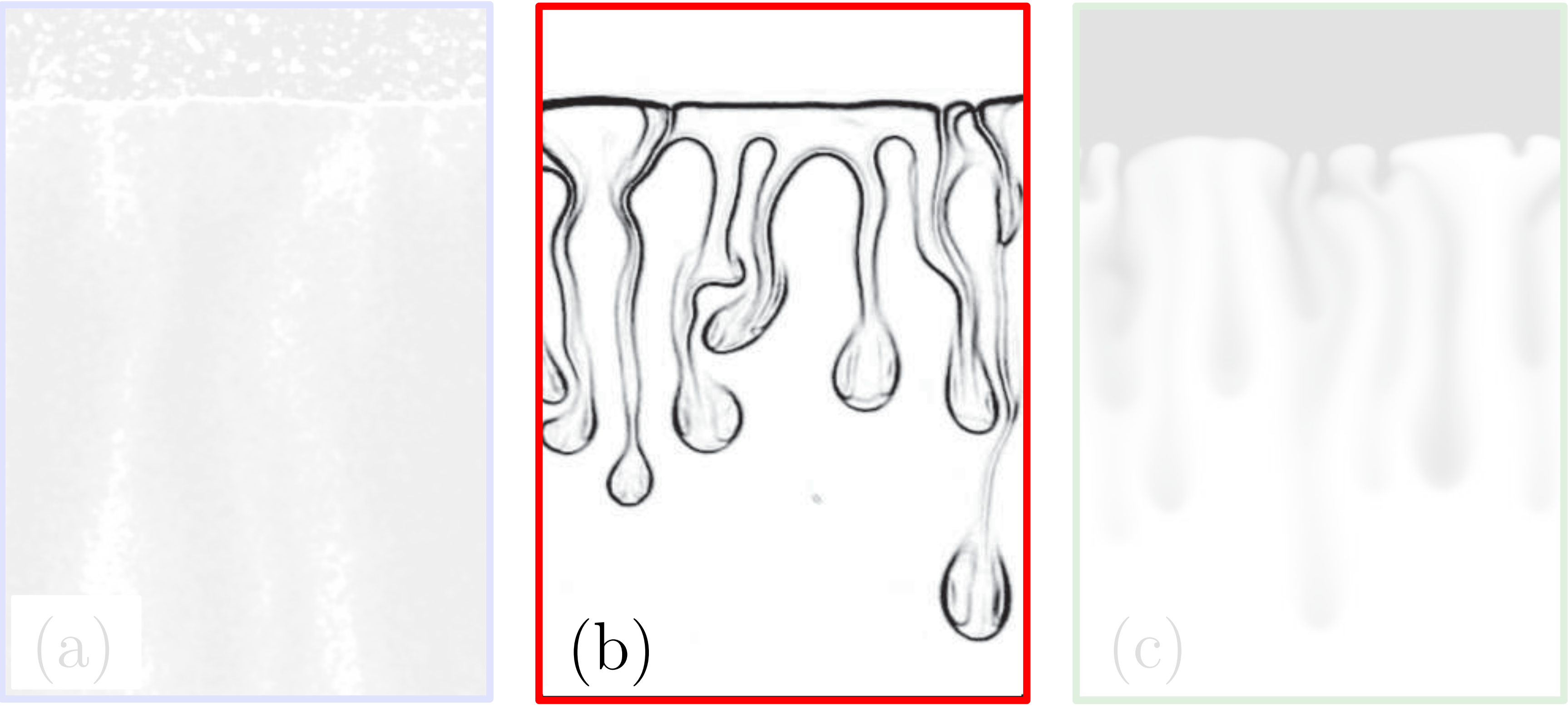

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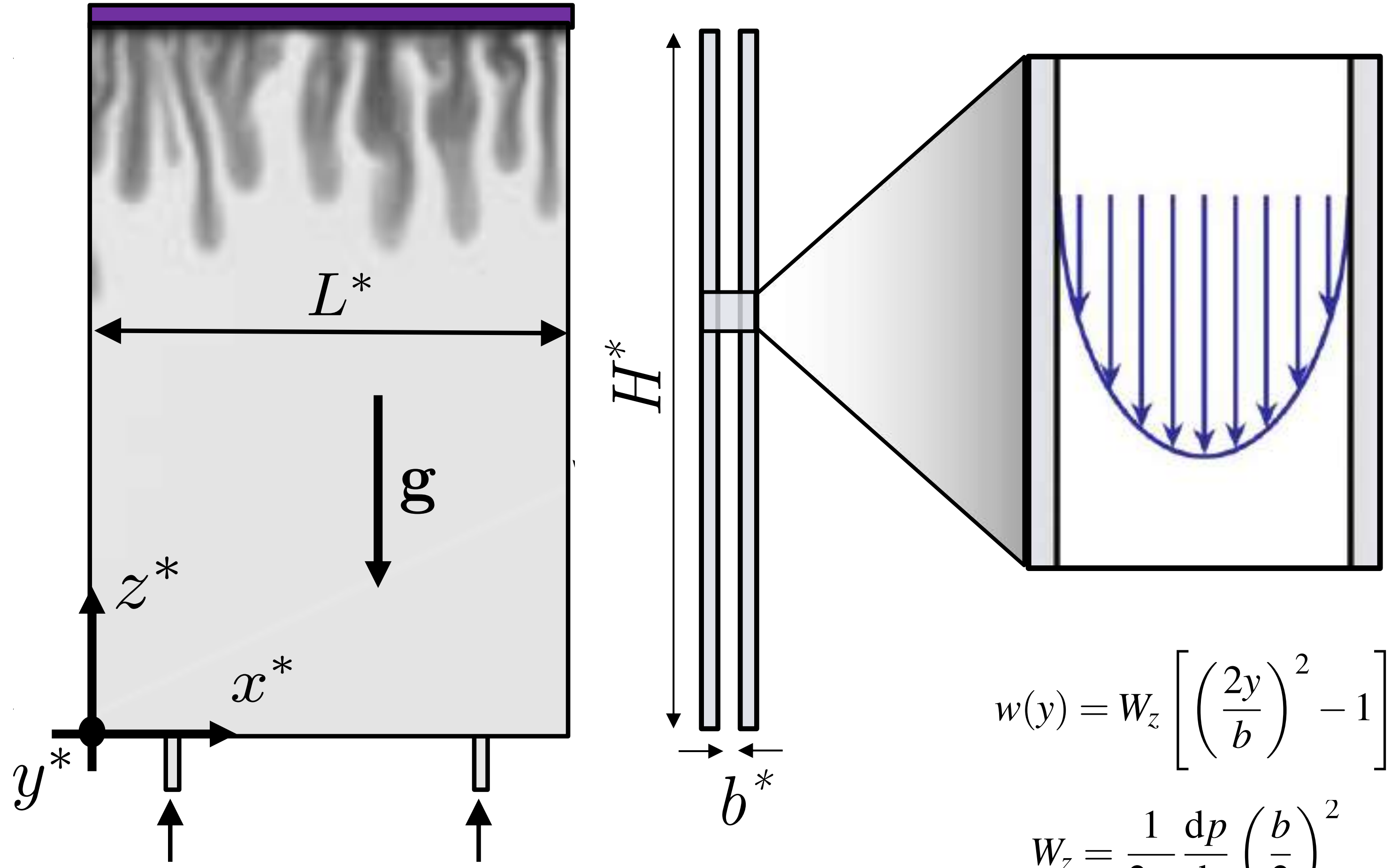
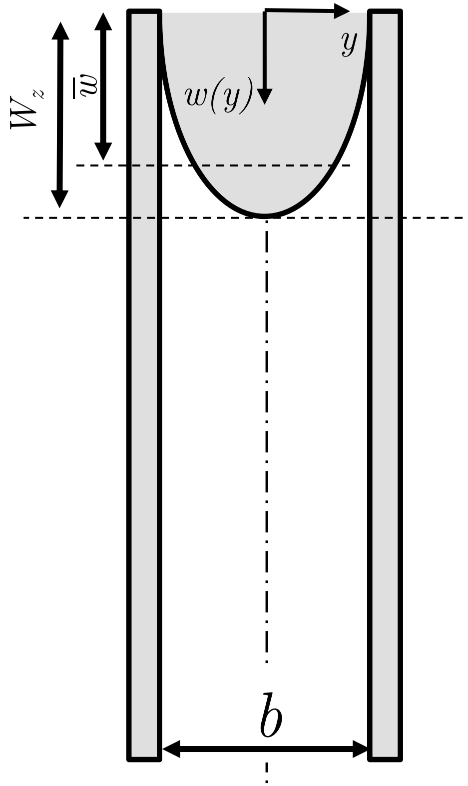


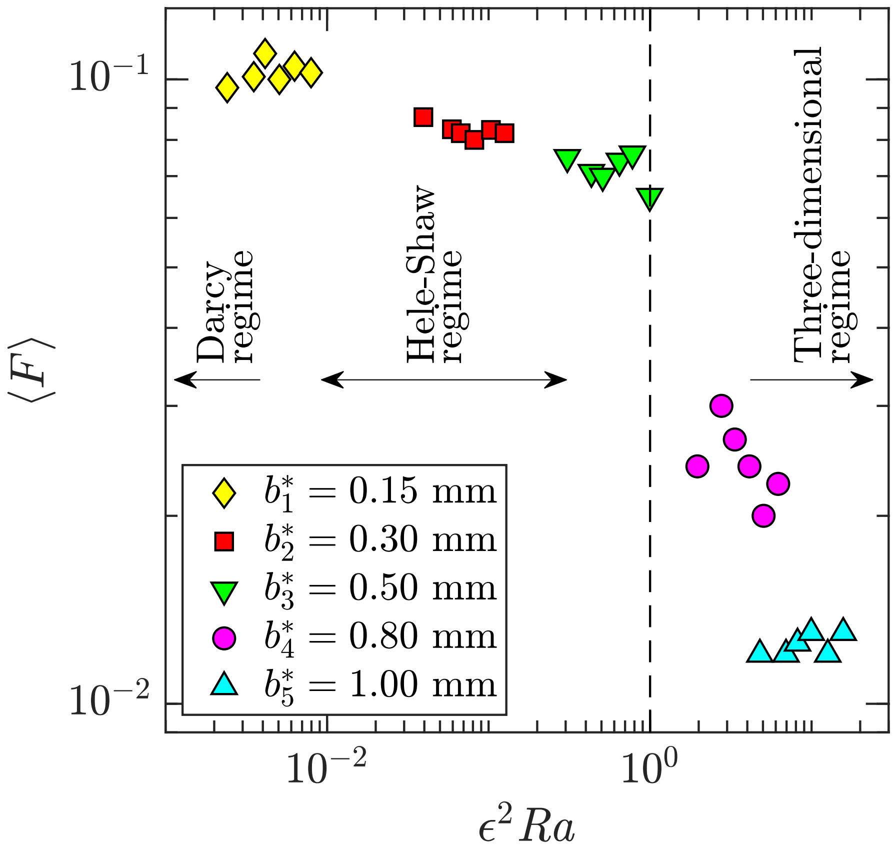
$$\overline{w} = \frac{2}{3} W_z = \frac{b^2/12}{\mu} \left| \frac{\mathrm{d}p}{\mathrm{d}z} \right|$$

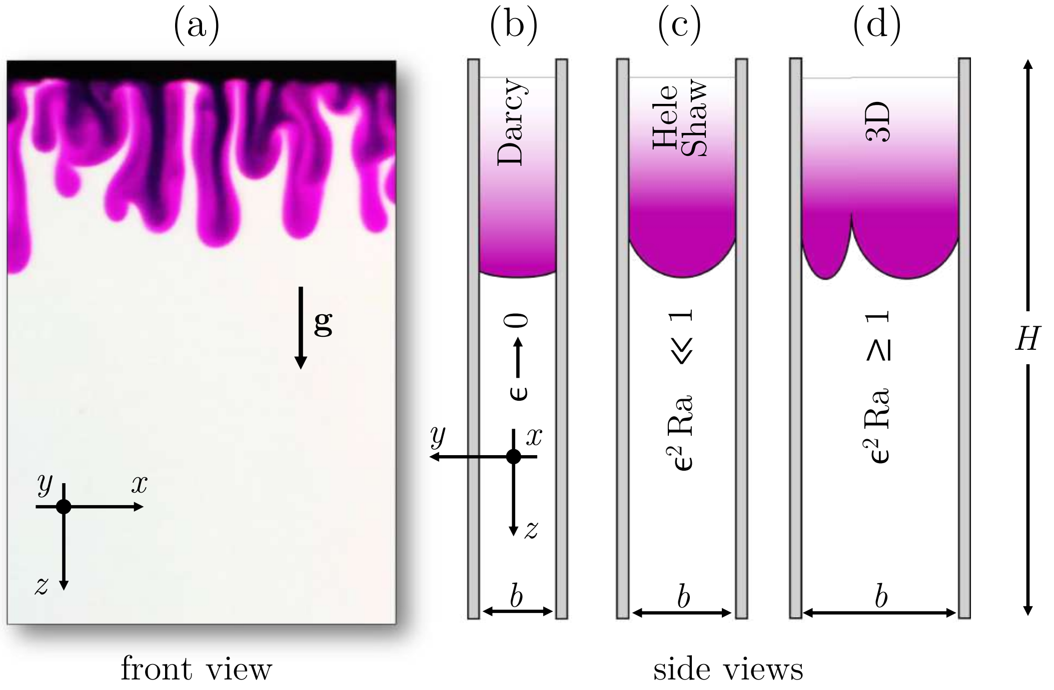


$$w(y) = W_z \left[\left(\frac{2y}{b} \right)^2 - 1 \right]$$

$$W_z = \frac{1}{2\mu} \frac{\mathrm{d}p}{\mathrm{d}z} \left(\frac{b}{2} \right)^2$$

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





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

De Paoli, Alipour & Soldati, *J. Fluid Mech.* (2020)

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

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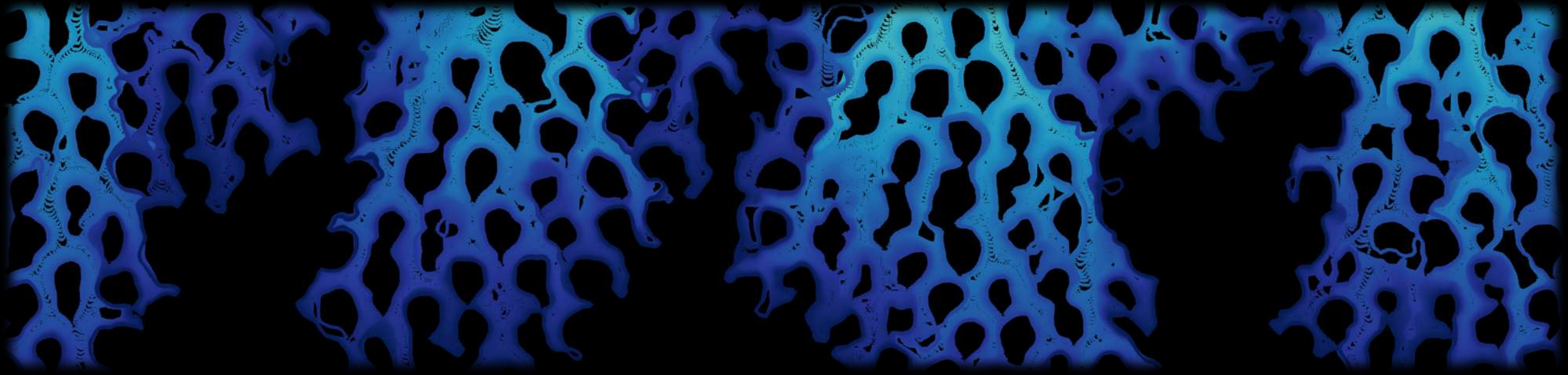

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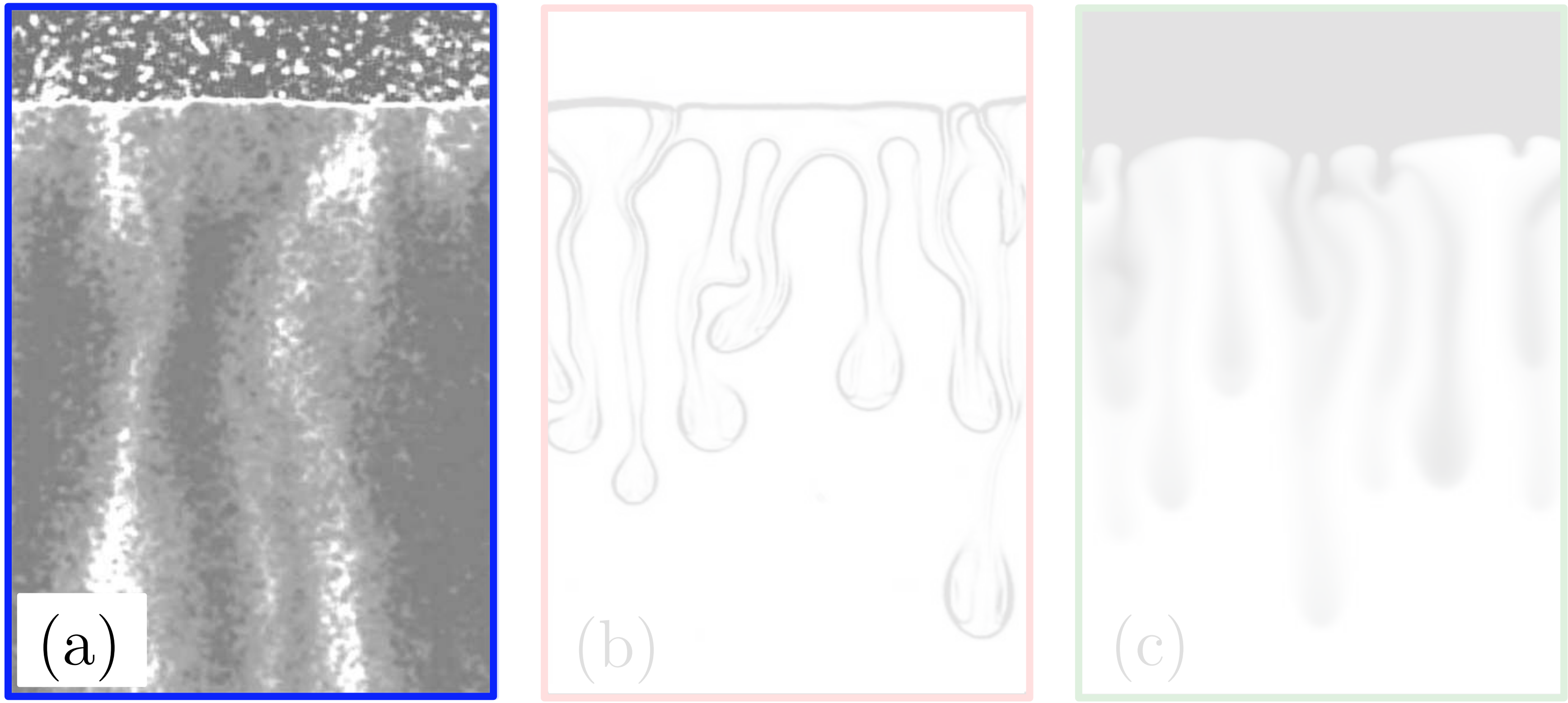

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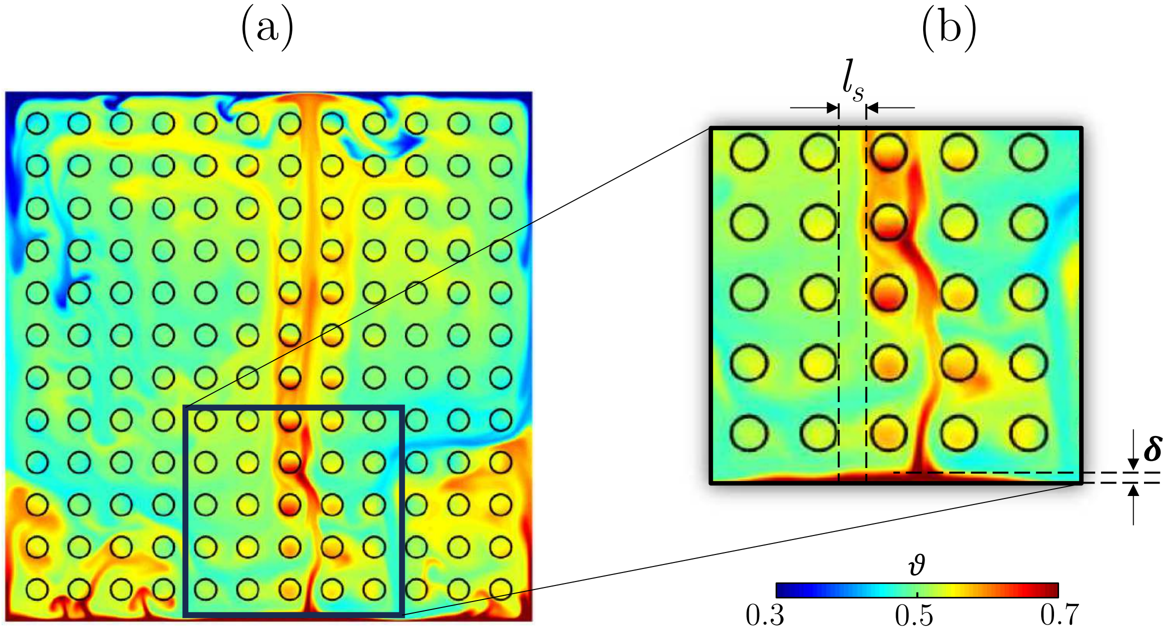
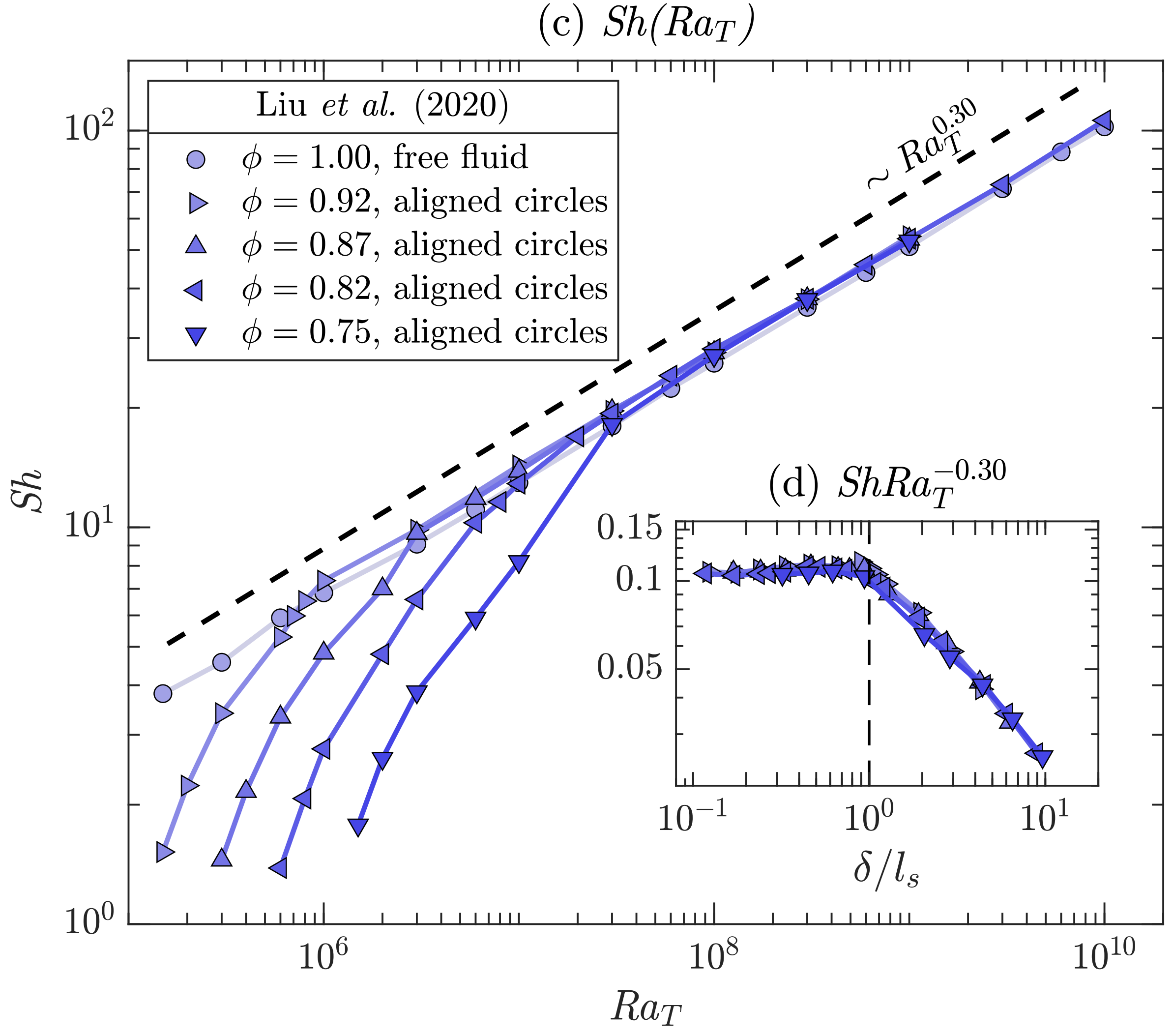
Pore-scale simulations

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





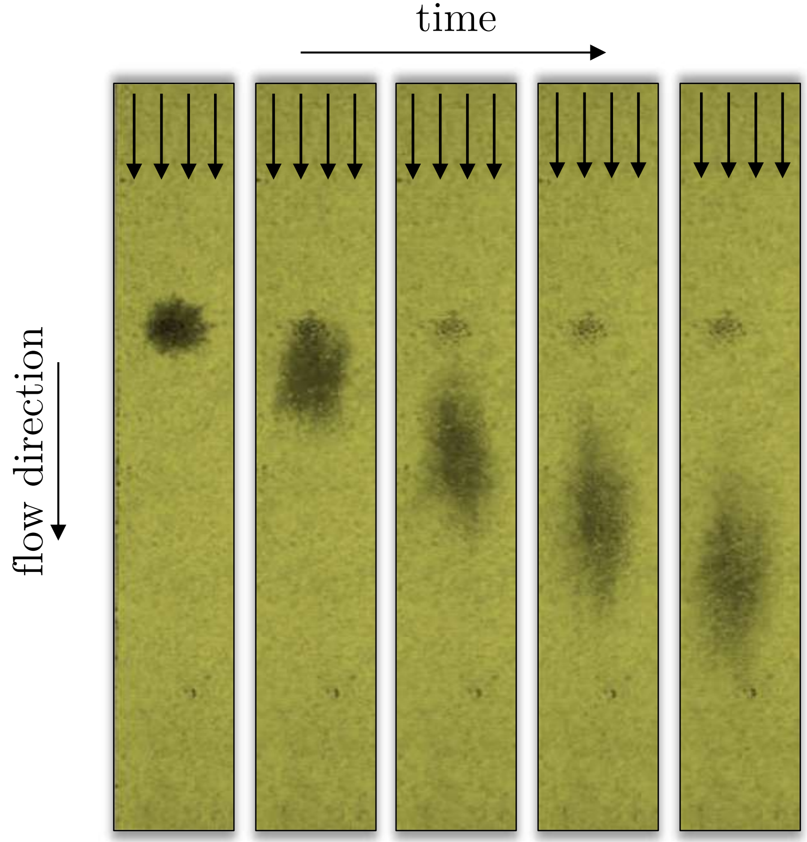
De Paoli, *Eur. Phys. J. E* (2023)

Liu et al., *J. Fluid Mech.* (2020)

Influence of dispersion

Mechanism of dispersion

Patch of dye in a uniform flow through a porous medium



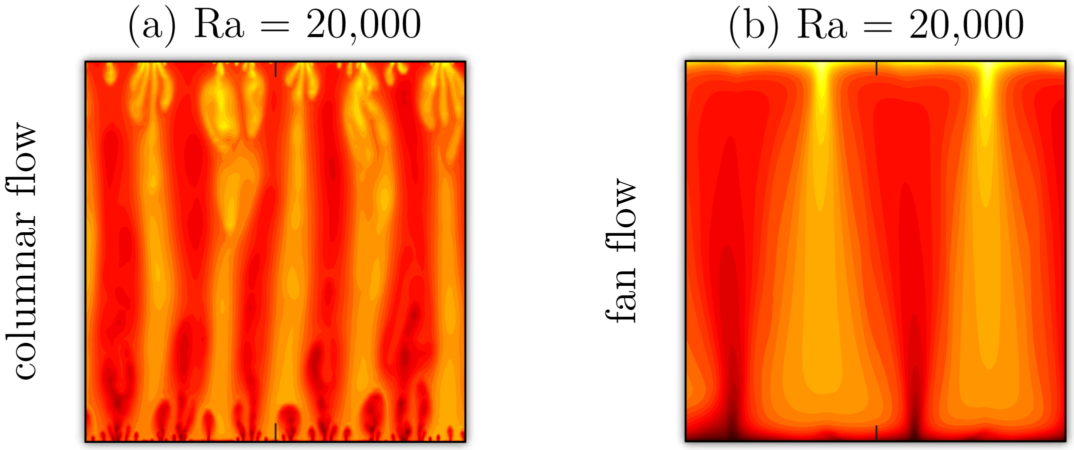
Woods, *Flows in porous rocks* (2015)

Darcy formulation of dispersion

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

Fickian formulation for dispersion

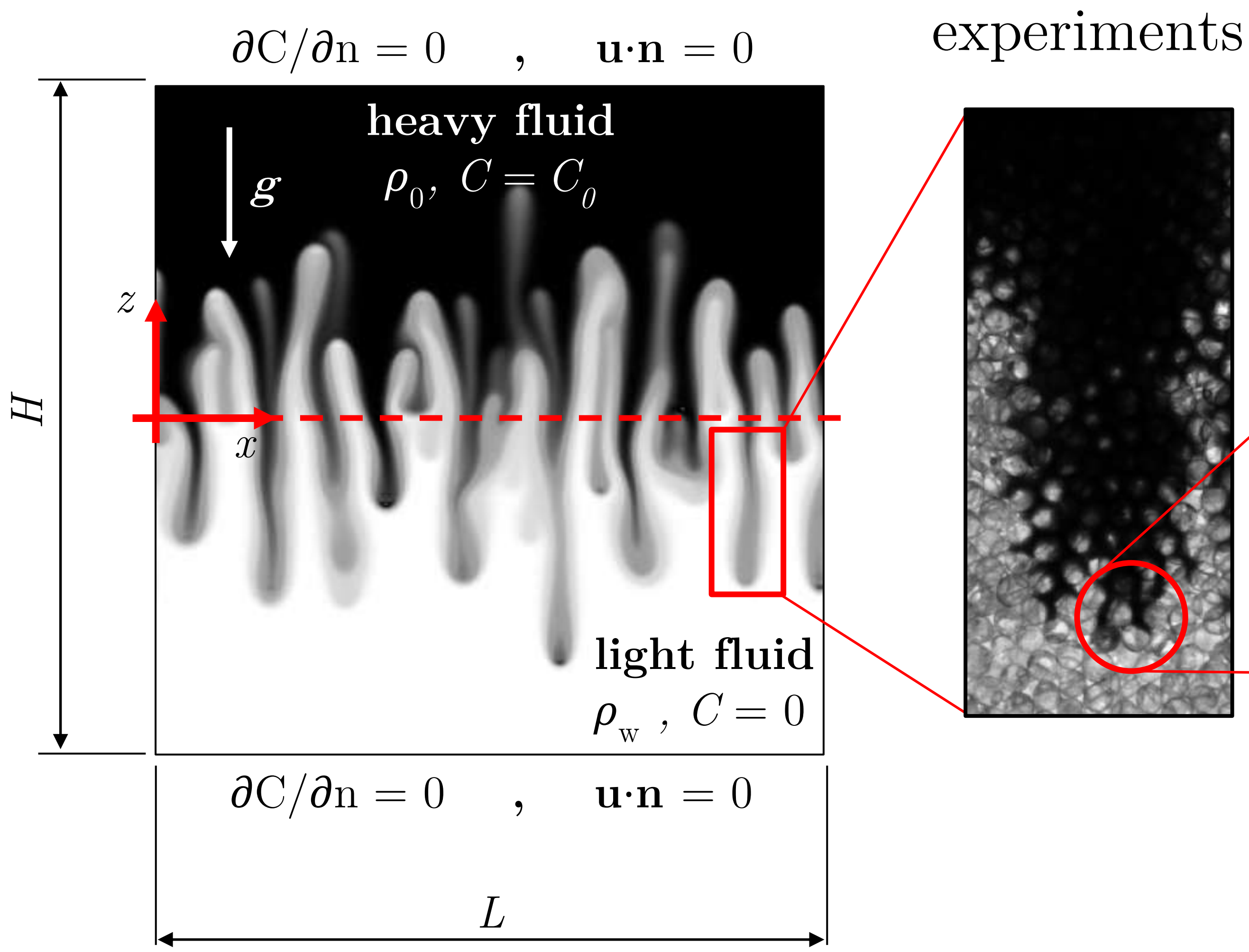
$$\mathbf{D}=D\mathbf{I}+(\alpha_L-\alpha_T)\frac{\mathbf{uu}}{|\mathbf{u}|}+\alpha_T\mathbf{uI},$$

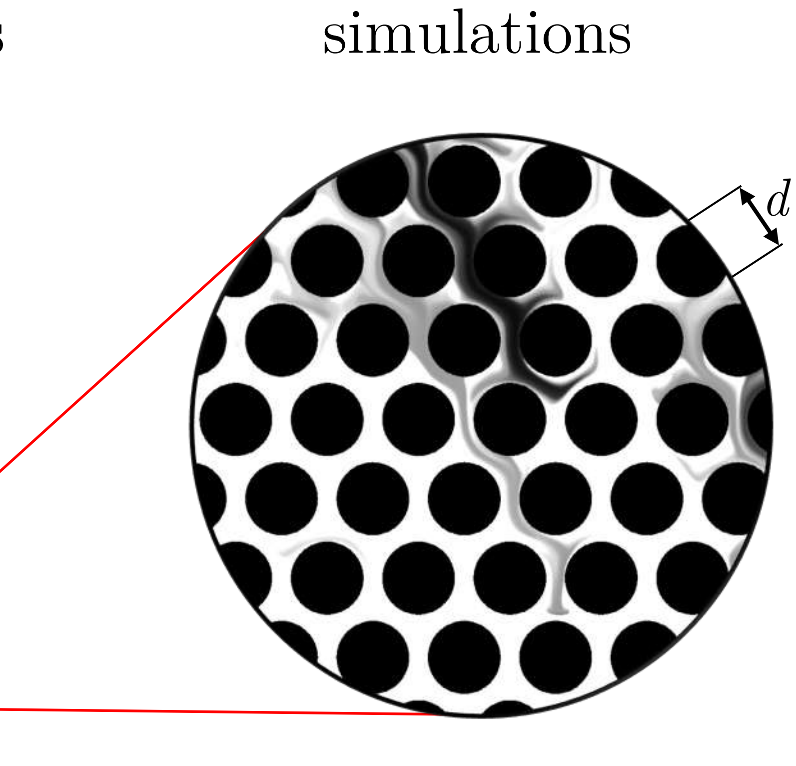


Liang et al., *Geophys. Res. Lett.* (2018)
Chang et al., *Phys. Rev. Fluids* (2018)

These models required validation: Experiments and simulations in porous media

Flow configuration

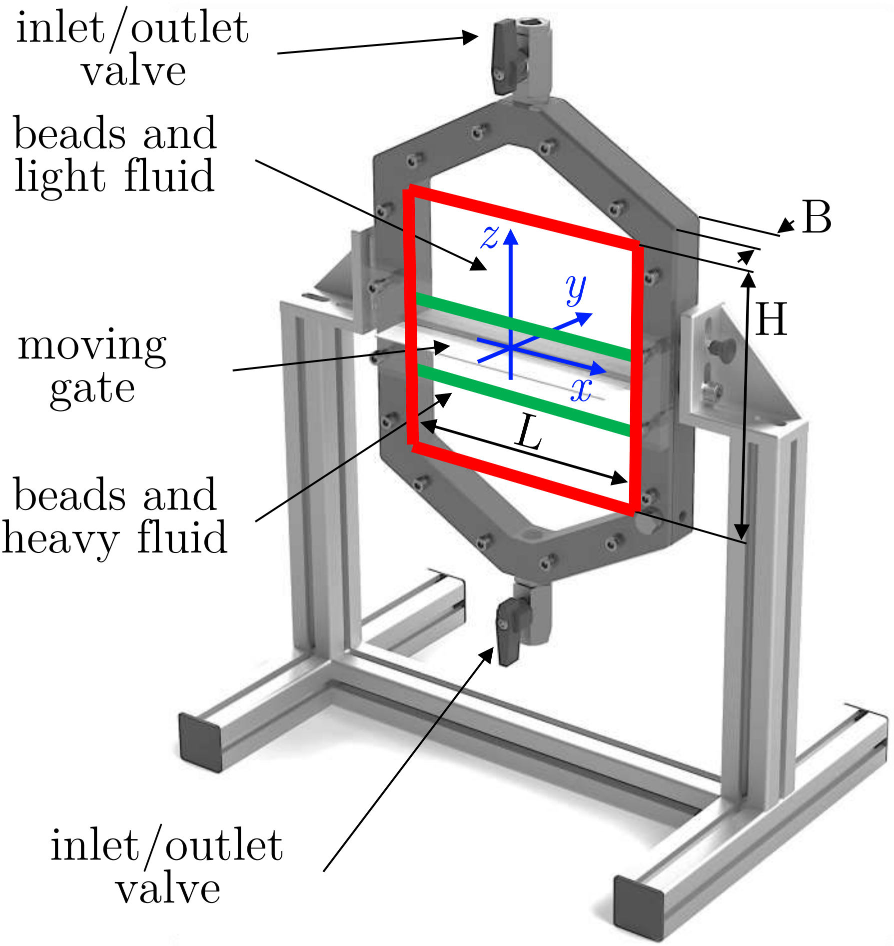




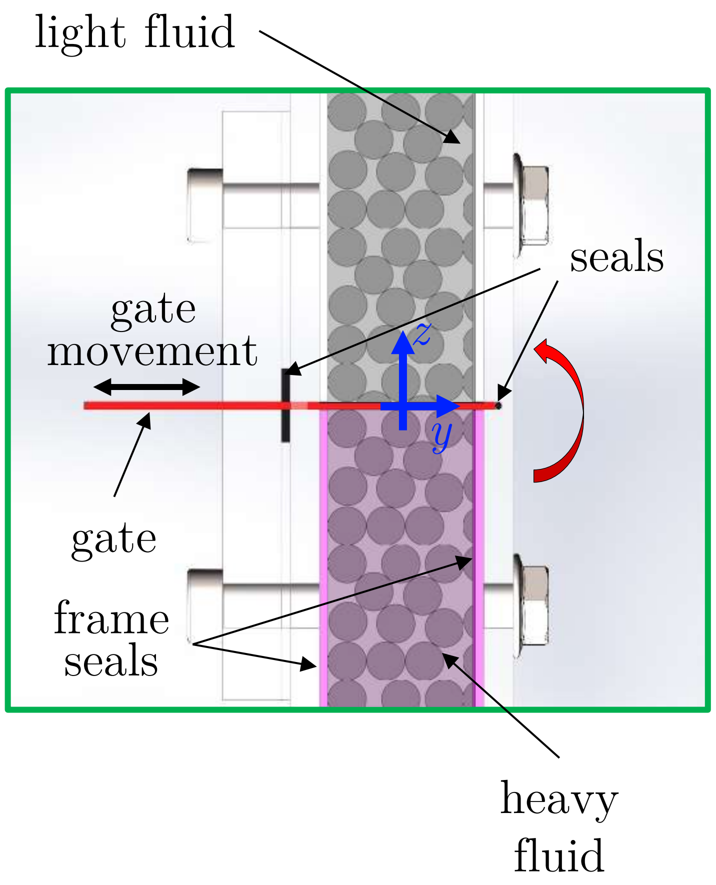
- High Schmidt number
- Porosity matched $\boldsymbol{\phi} = 0.37$
- Solid impermeable to solute
- Linear dependency $\rho(C)$

Experimental setup

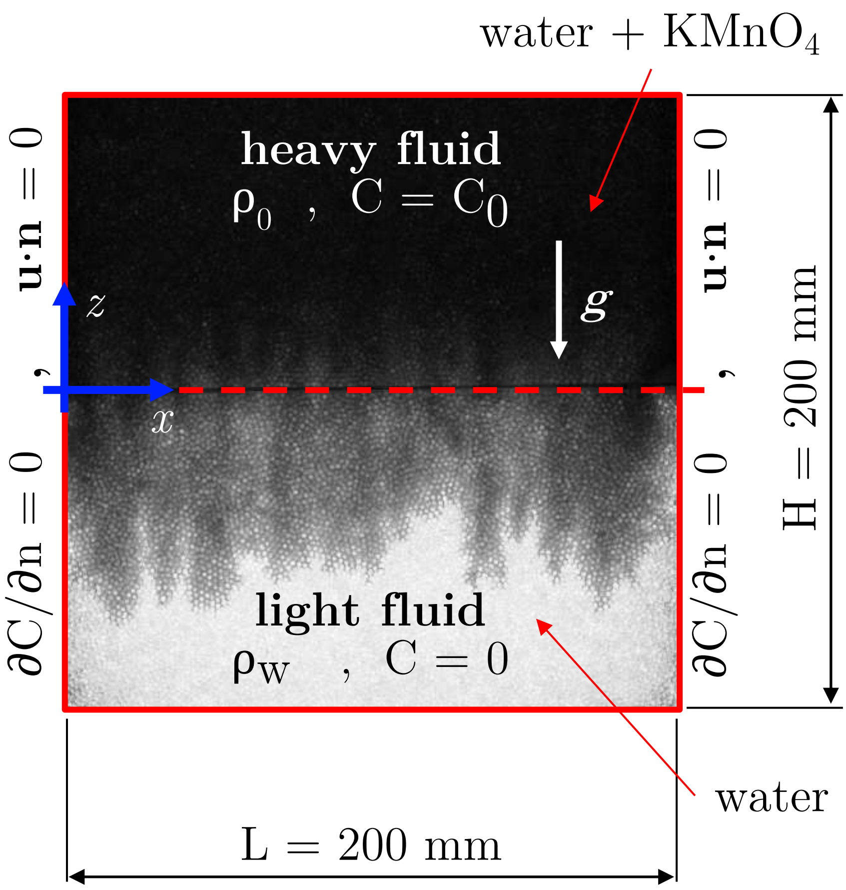
(a) Hele-Shaw cell

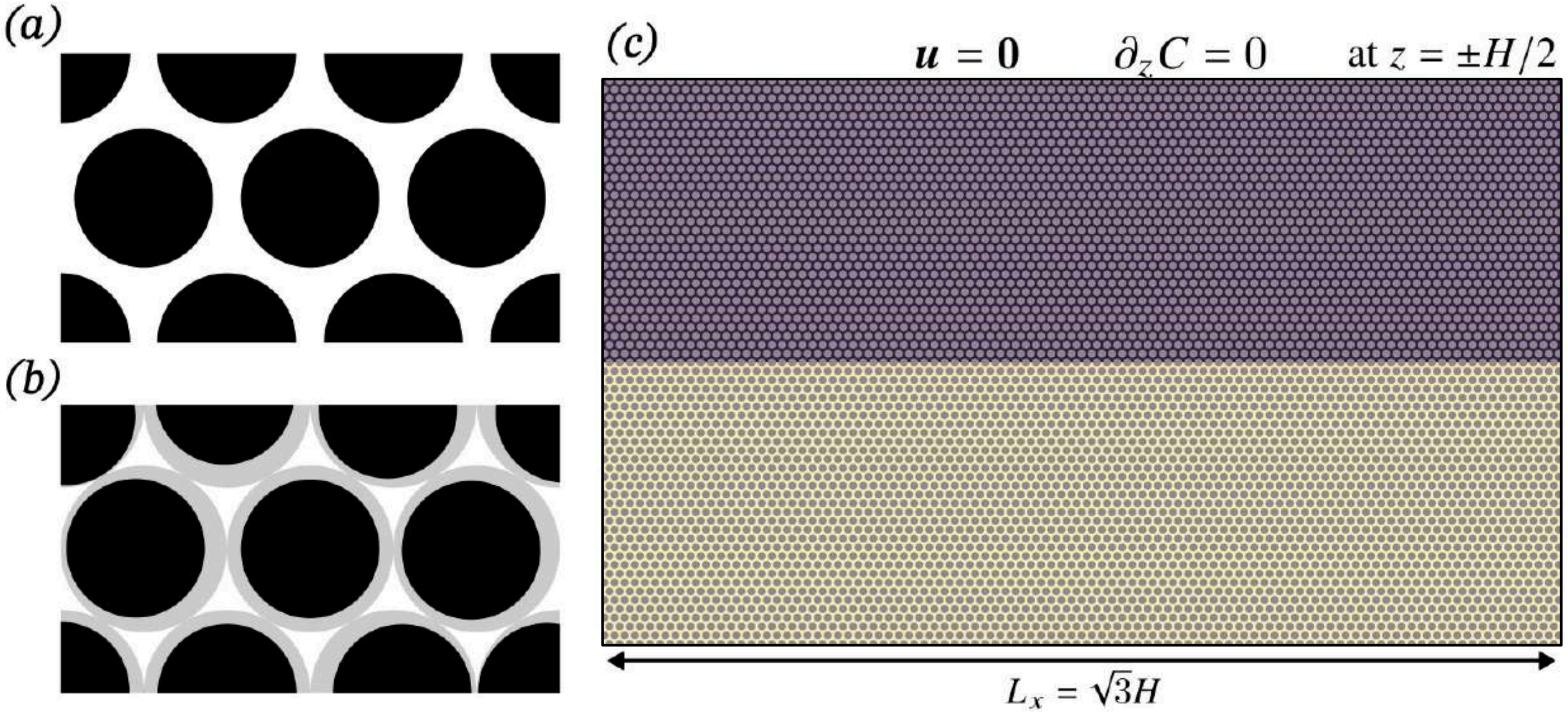


(b) gate (side view)



(c) measurement region





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

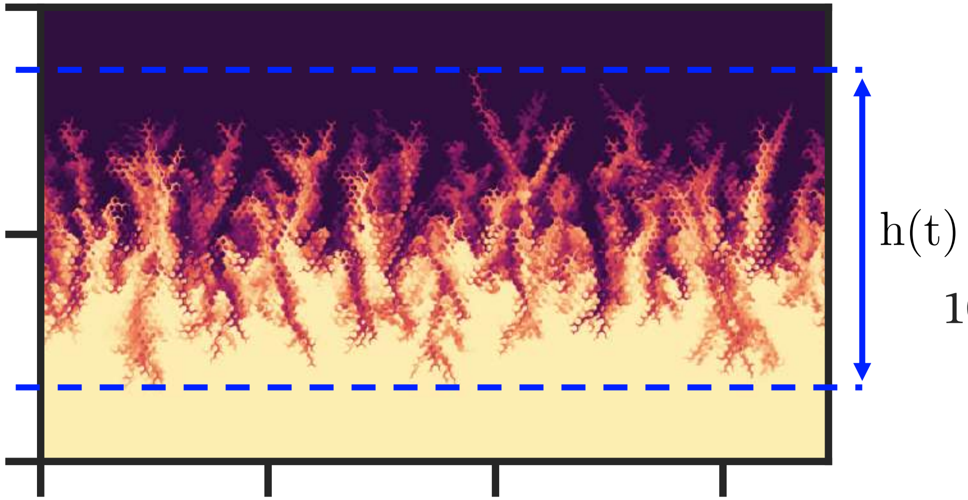
$$\partial_t C + (\boldsymbol{u} \cdot \boldsymbol{\nabla})C = D\nabla^2 C,$$

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

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

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

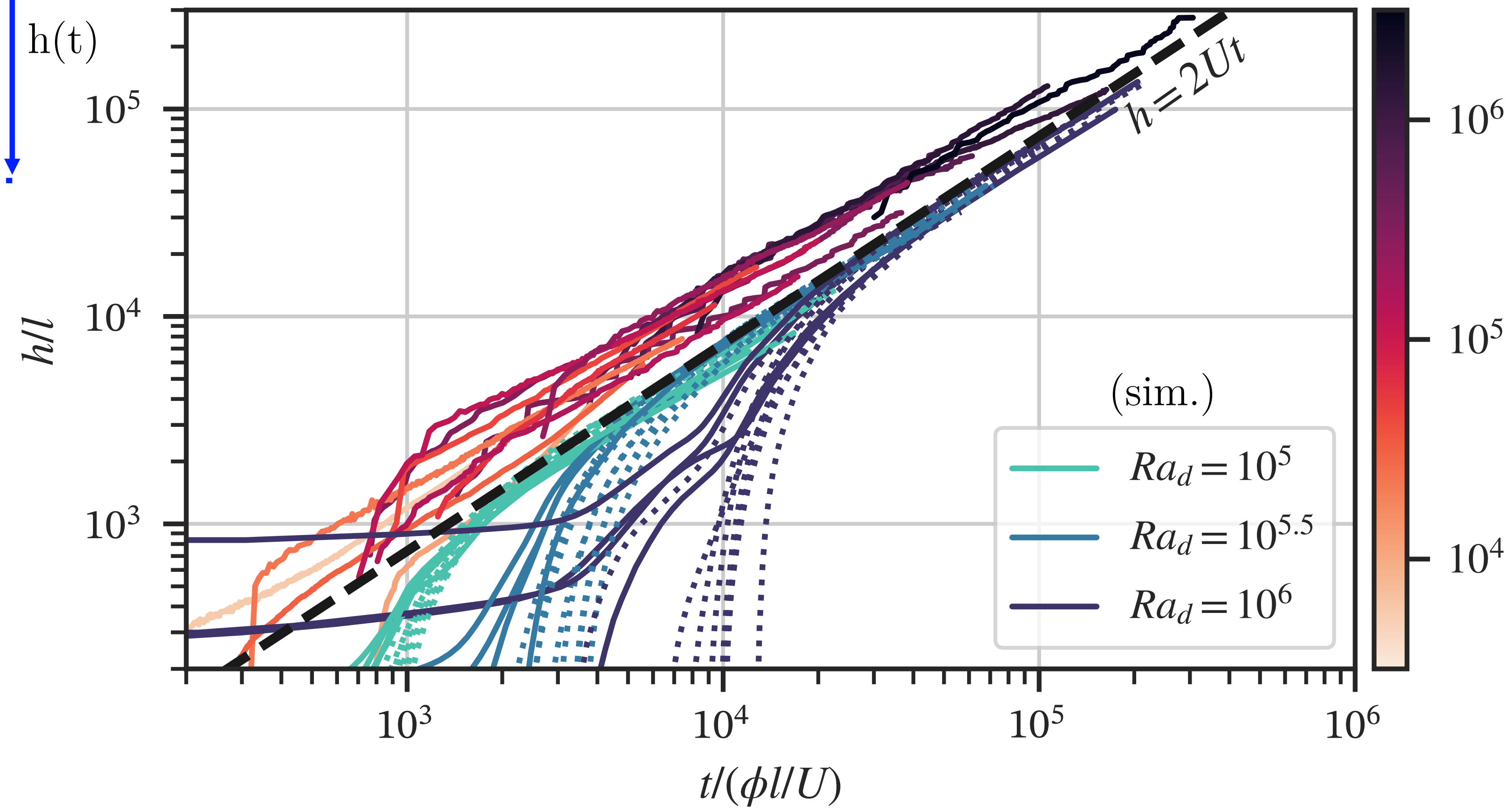
Mixing length



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

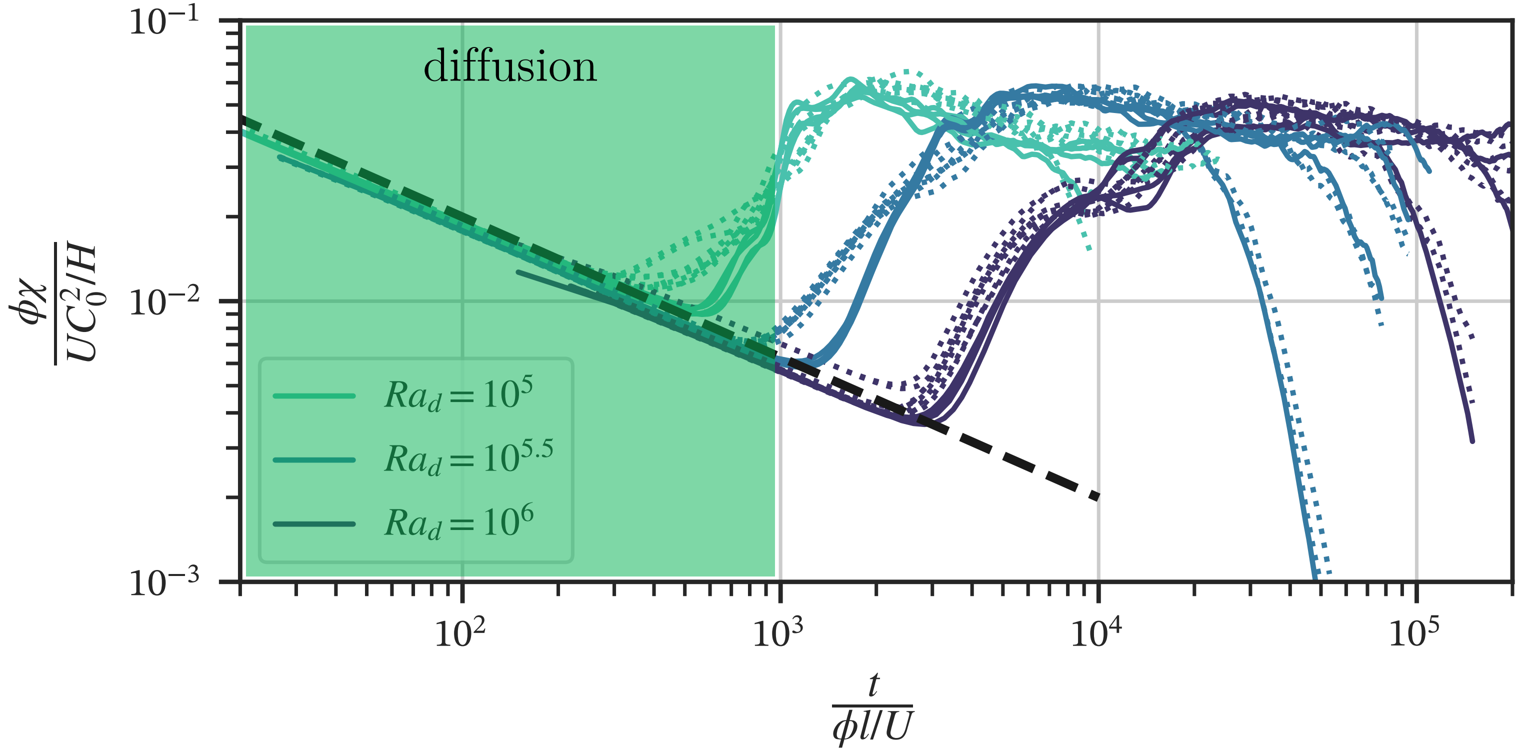
$$\ell = \frac{\phi D}{U}$$

$$Ra_d = \frac{g\Delta\rho d^3}{\mu D}$$



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

Can we model this mixing/dissolution process?



Diffusion:

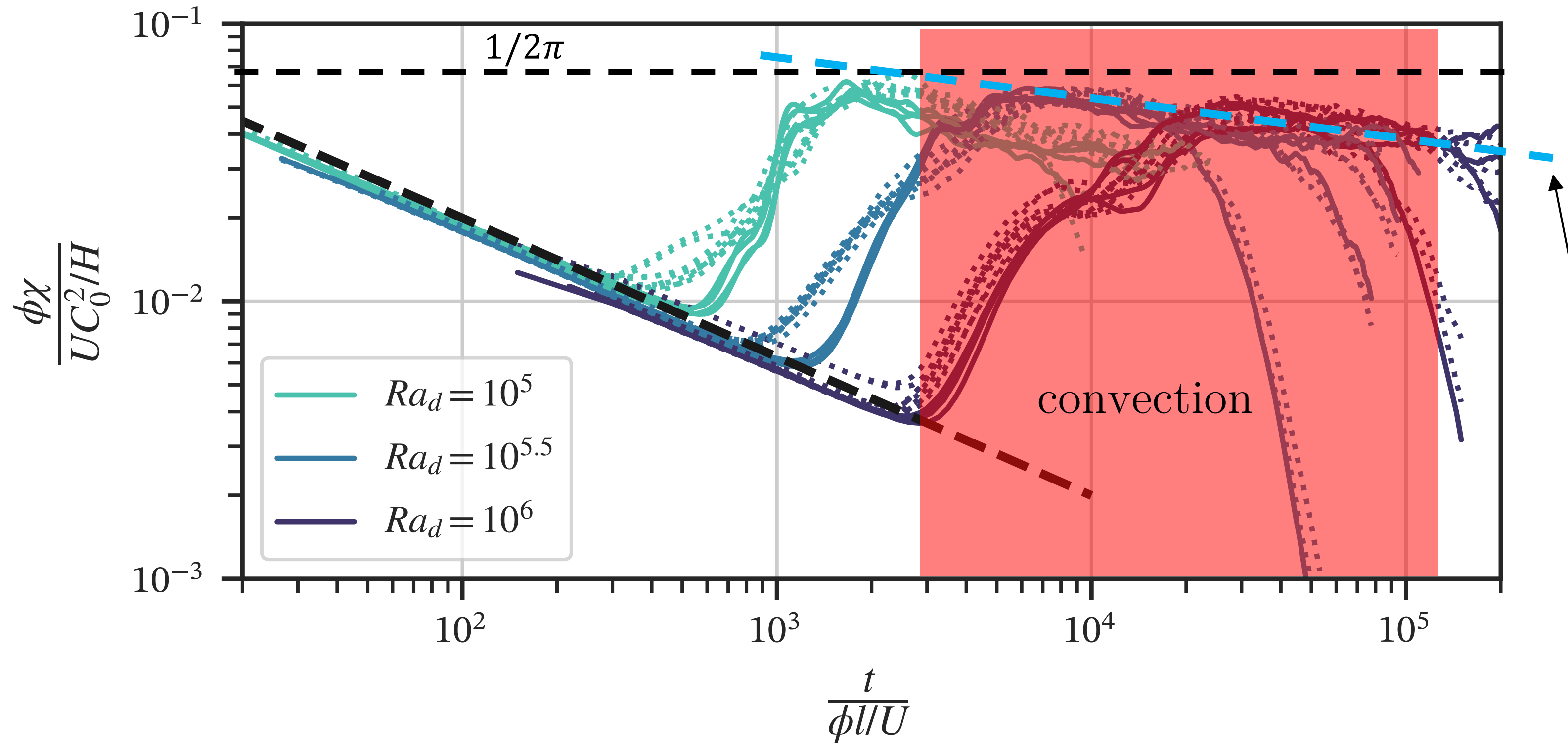
$$C = C_0 + \frac{\Delta C}{2}\mathrm{erf}\left(\frac{z}{\sqrt{2\kappa t}}\right)$$

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

$$\chi = \kappa\langle|\nabla C|^2\rangle = \frac{\kappa}{H}\int_{-\infty}^{\infty}|\partial_z C|^2 \mathrm{d}z$$

$$= \sqrt{\frac{\kappa}{8\pi t}}\frac{(\Delta C)^2}{H}$$

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



Convection

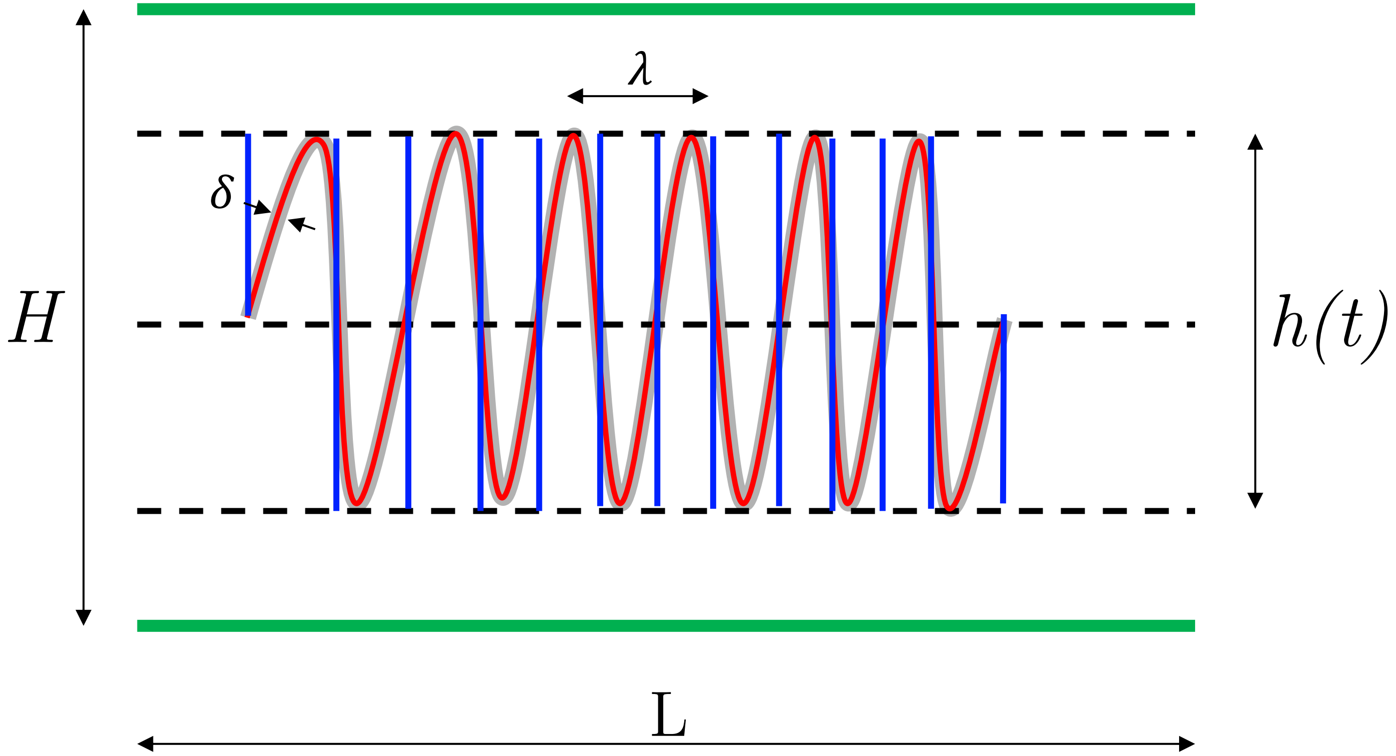
$$\chi = \kappa\langle|\nabla C|^2\rangle = \kappa\frac{L_m}{H}\langle|\nabla C|^2\rangle_{ML},$$

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

$$L_m \approx 2Ut,$$

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

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



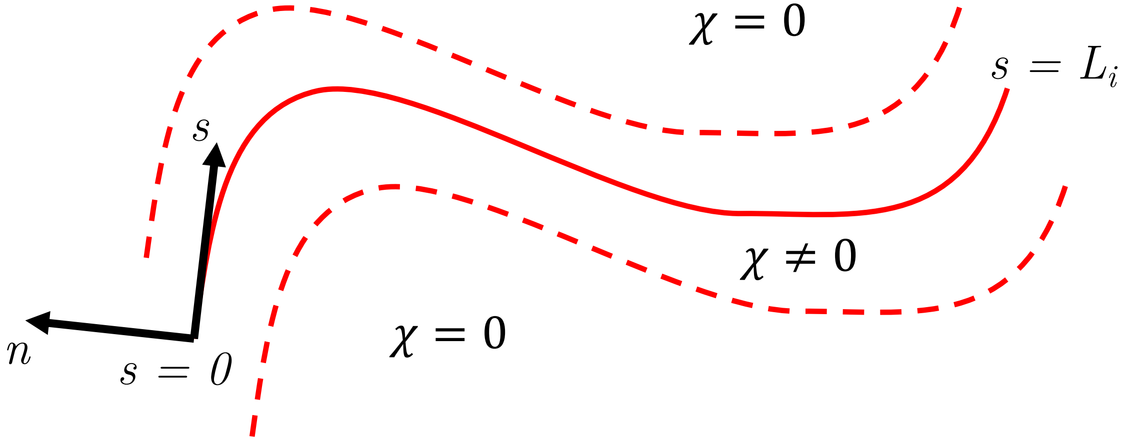
$$\chi = D\langle|\nabla C|^2\rangle = \frac{D L_i}{HL}\int_{-\delta/2}^{+\delta/2} |\partial_n C|^2 \, dn$$

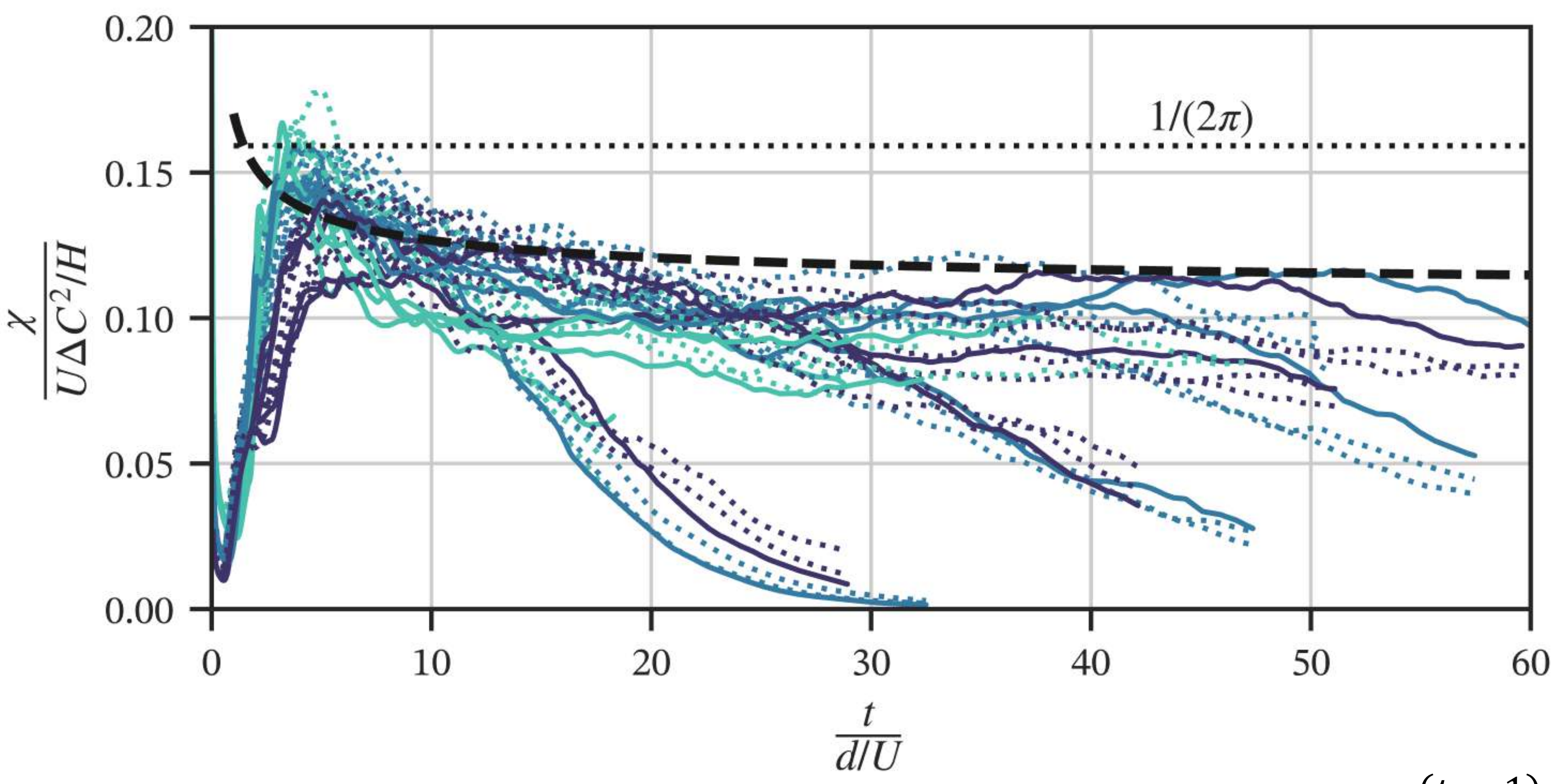
Assume:

1) Interface grows as:

$$L_i = L + 2\,N_{finger}\,h = L + 2\frac{L}{\lambda}h$$

2) Gradient across the interface evolves according to the diffusive solution



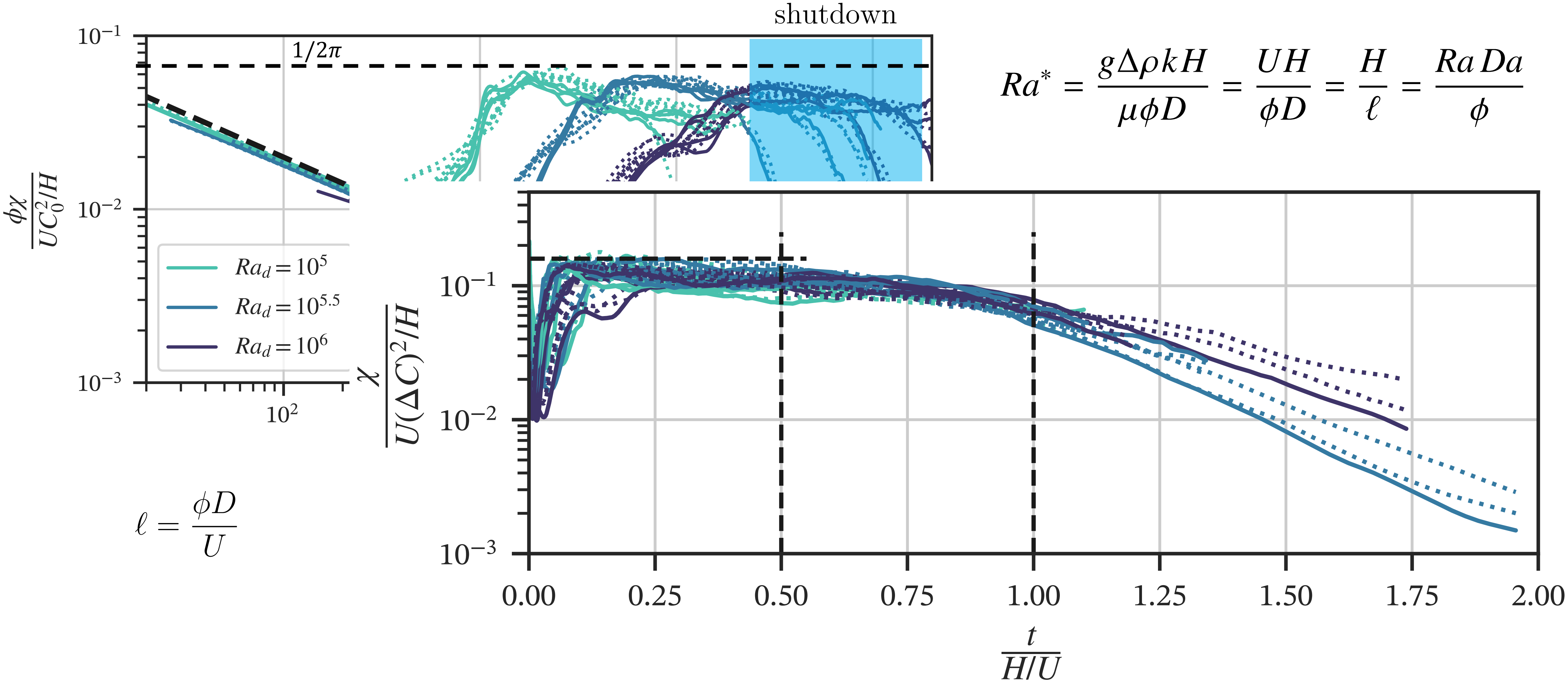


$1/2\pi$ is the maximum value of dissipation.

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

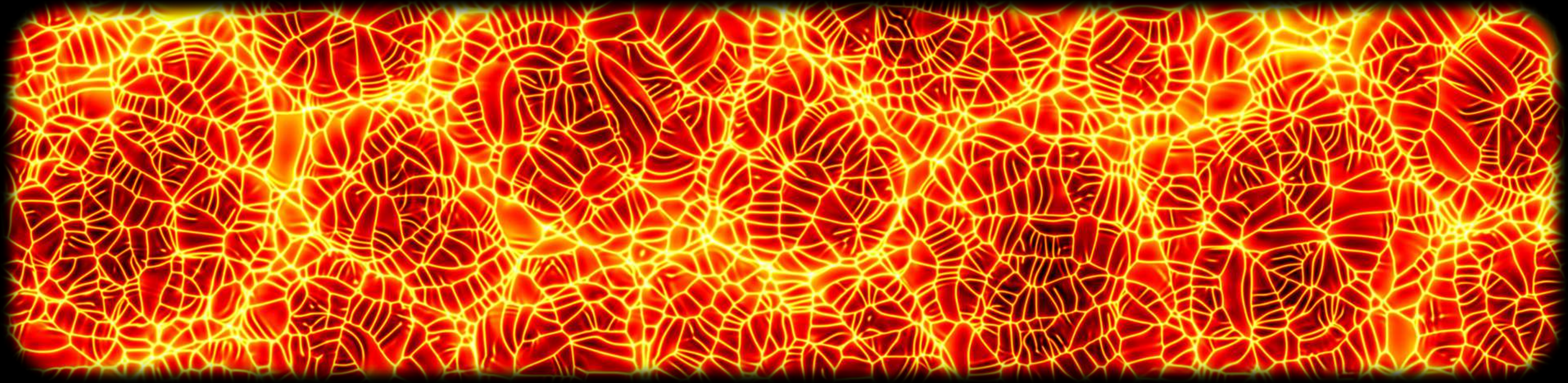
$$\frac{\chi(t=1)}{(\Delta C)^2 U/H} = \frac{\beta}{\alpha\pi}\left(1+\frac{\alpha}{4}\right) \approx \frac{1}{1.92\pi} \approx \frac{1}{2\pi}$$

Modelling scalar dissipation

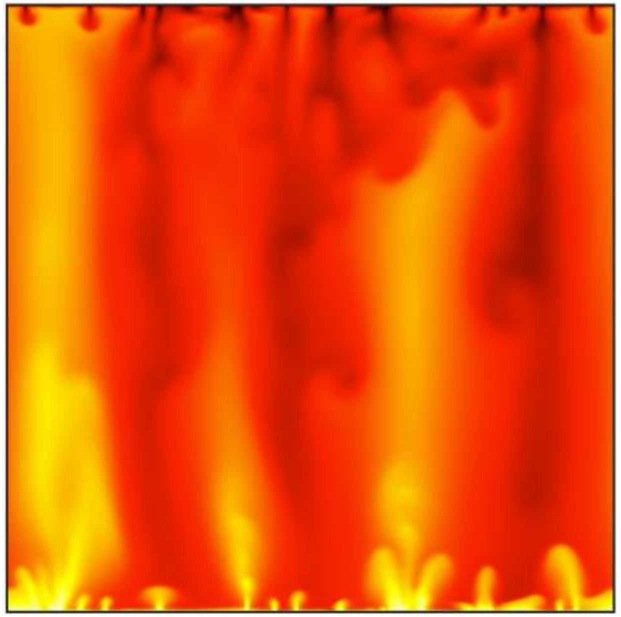


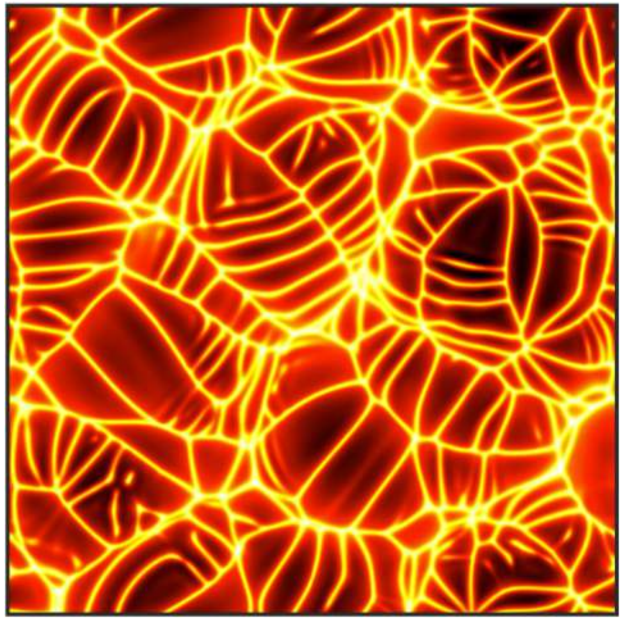
$$Ra^* = \frac{g\Delta\rho k H}{\mu\phi D} = \frac{UH}{\phi D} = \frac{H}{\ell} = \frac{Ra\,Da}{\phi}$$

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



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

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