Multiscale modelling of convective mixing in confined porous media

M. De Paoli[1,2]

m.depaoli@utwente.nl

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

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

Physics of Fluids

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A. Soldati

F. Zonta

V. Giurgiu

M. Alipour

SAPIENZA UNIVERSITÀ DI ROMA

S. Pirozzoli

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

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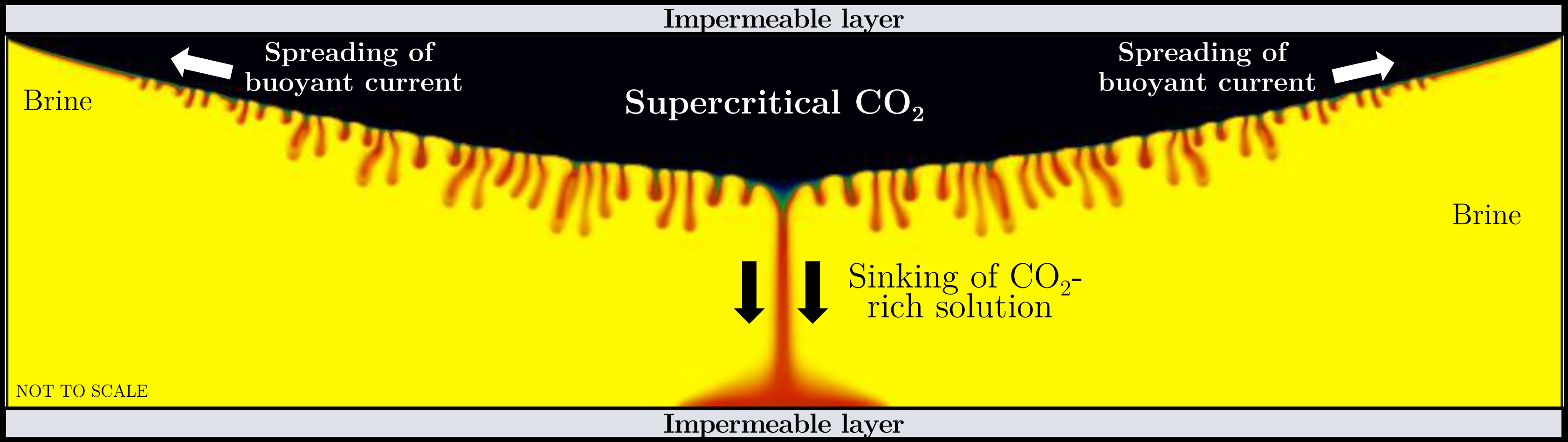
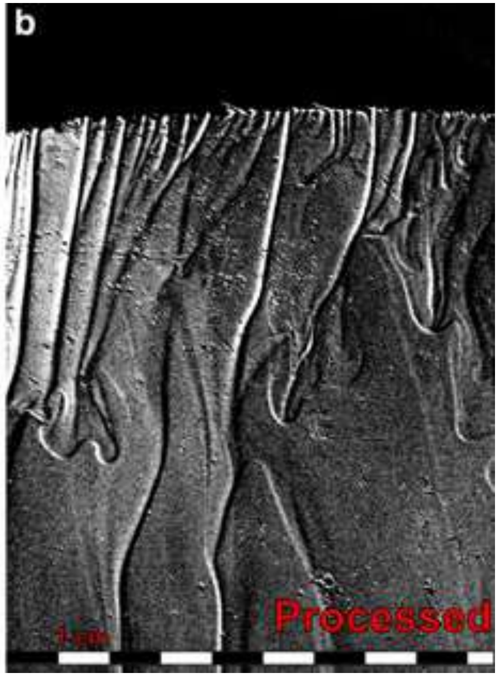
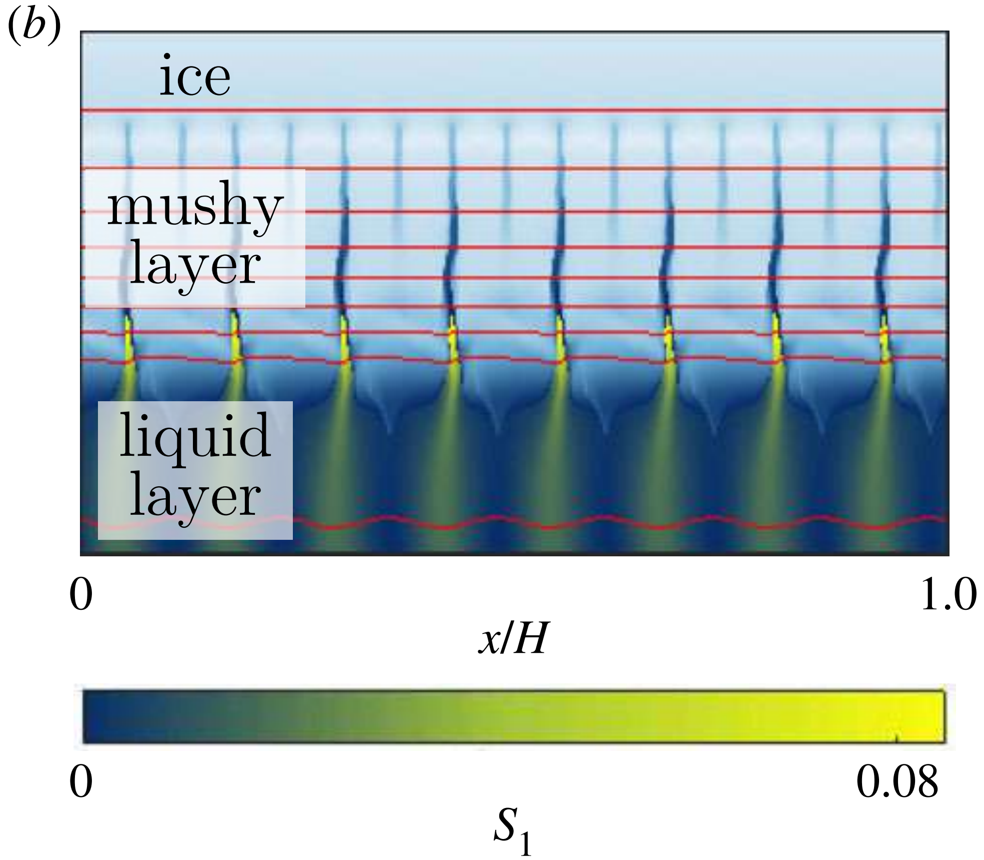


Sea ice formation



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



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

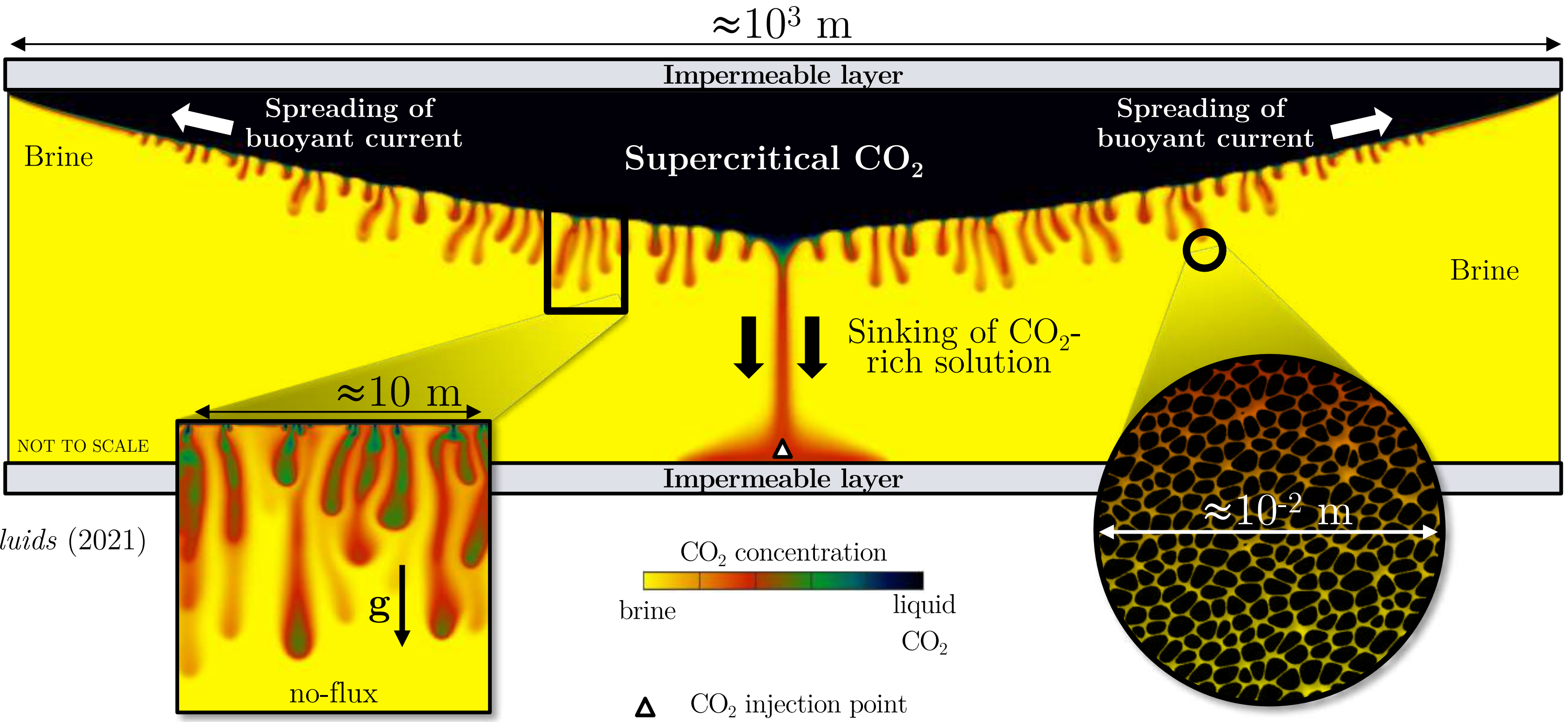
Other applications

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).

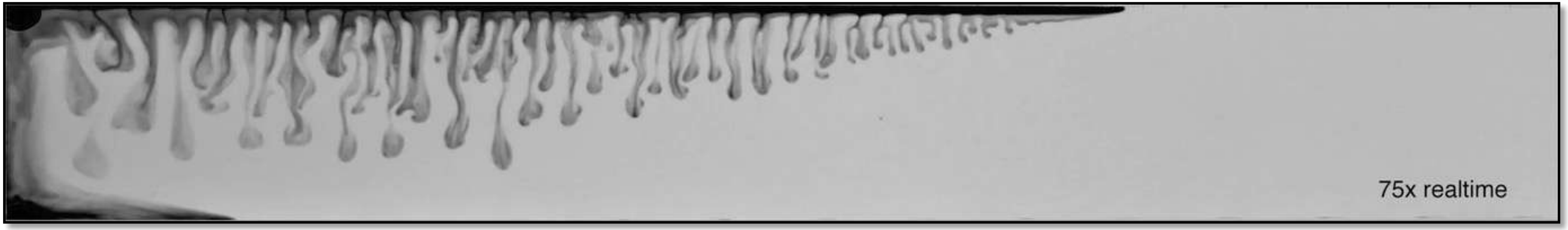
LeBlanc, *Sewage plume in a sand and gravel aquifer, Cape Cod, Massachusetts* (US Geological Survey, 1984).

Carbon Capture and Storage



De Paoli, *Phys. Fluids* (2021)

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



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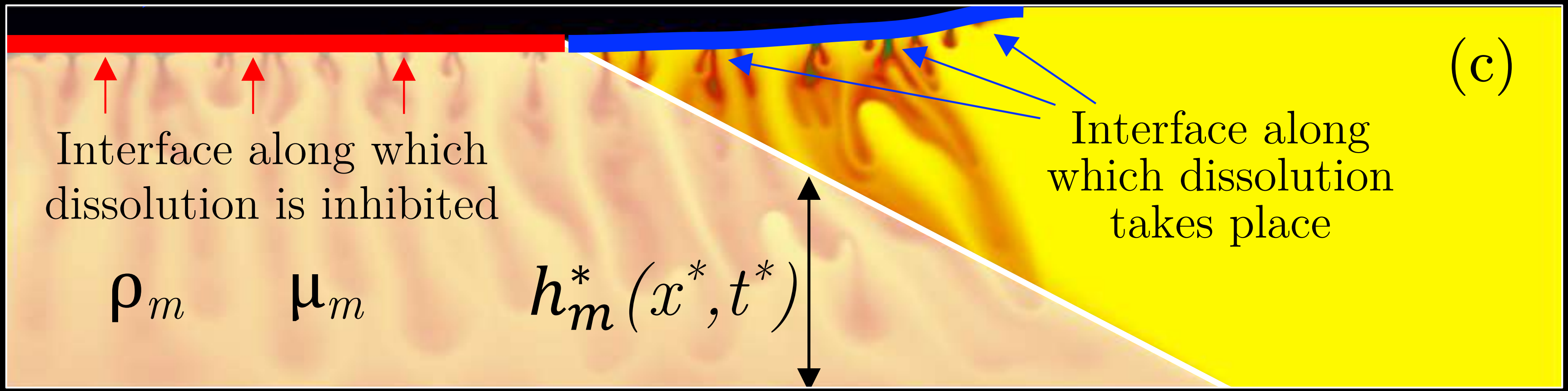
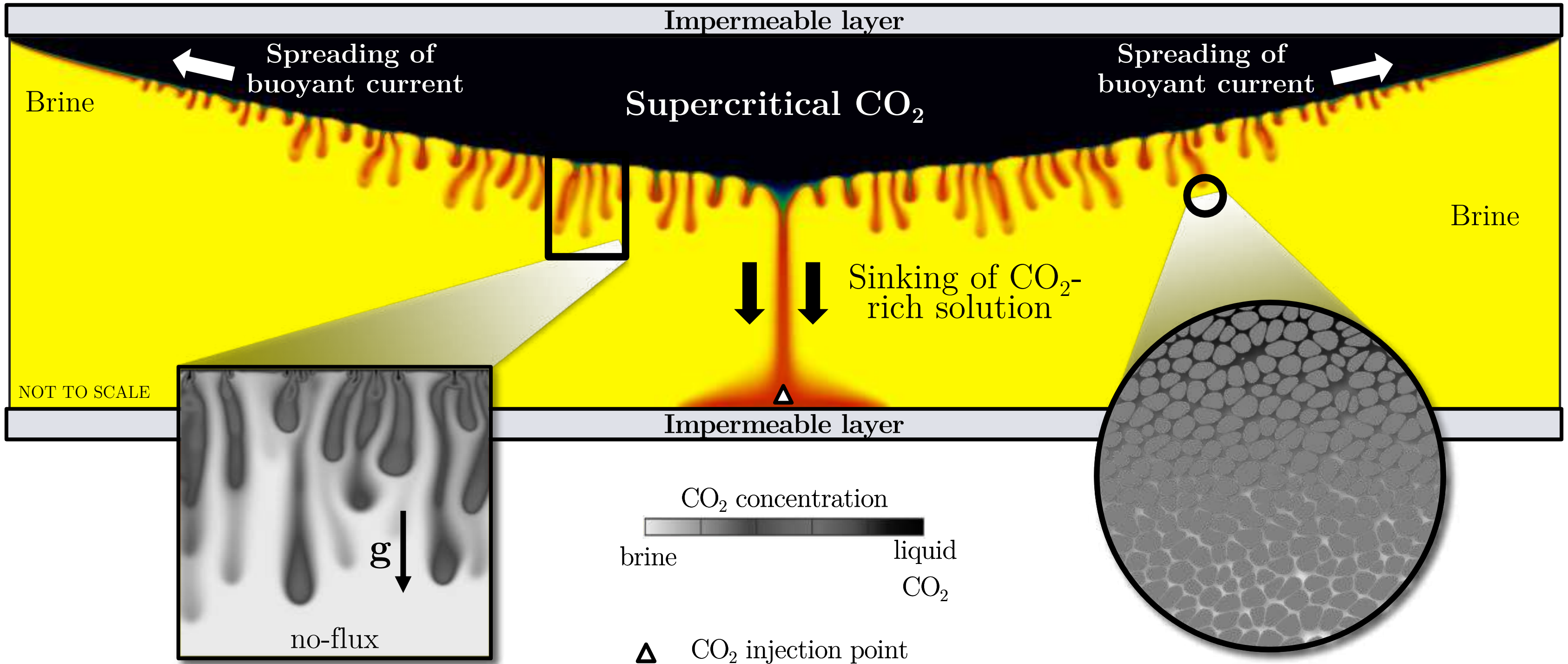


Carbon Capture and Storage

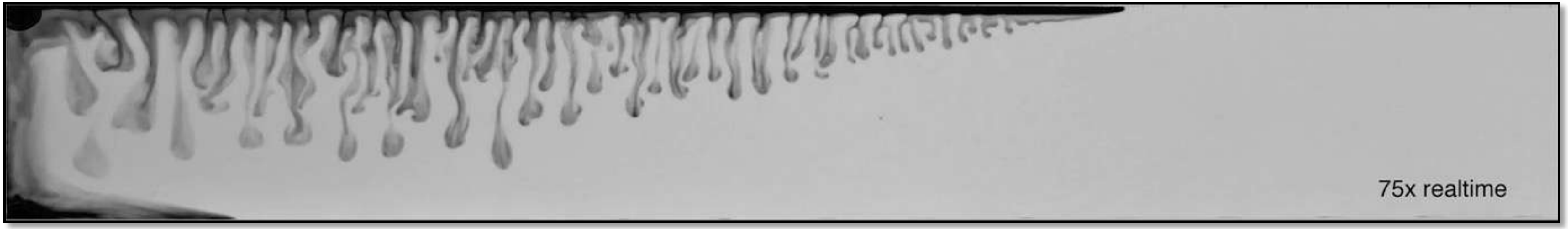


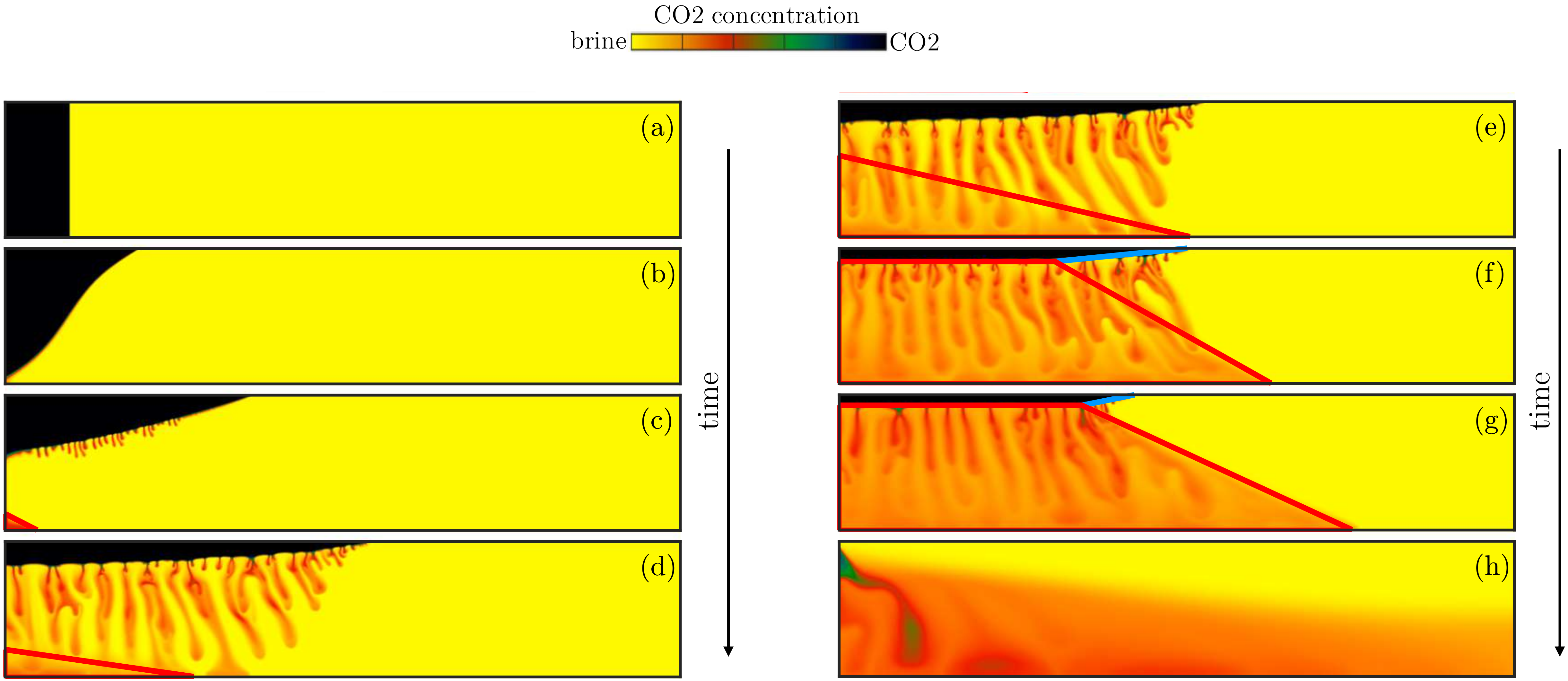
De Paoli, *Phys. Fluids* (2021)

Reservoir properties

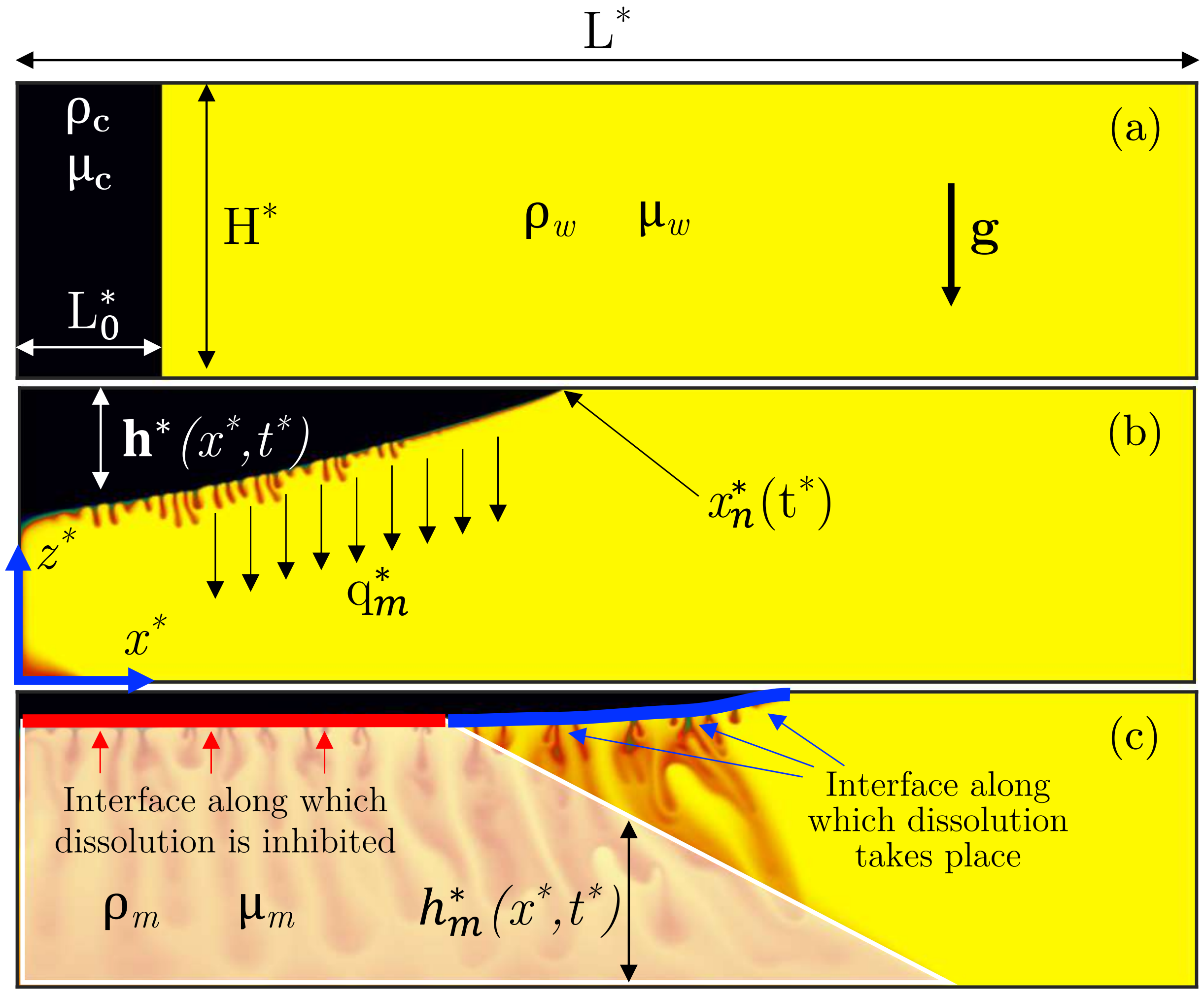
- anisotropy and heterogeneities
- finite size of confining layers
- effects of rock properties (mechanical dispersion)
- chemical dissolution and morphology variations
- ...

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





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

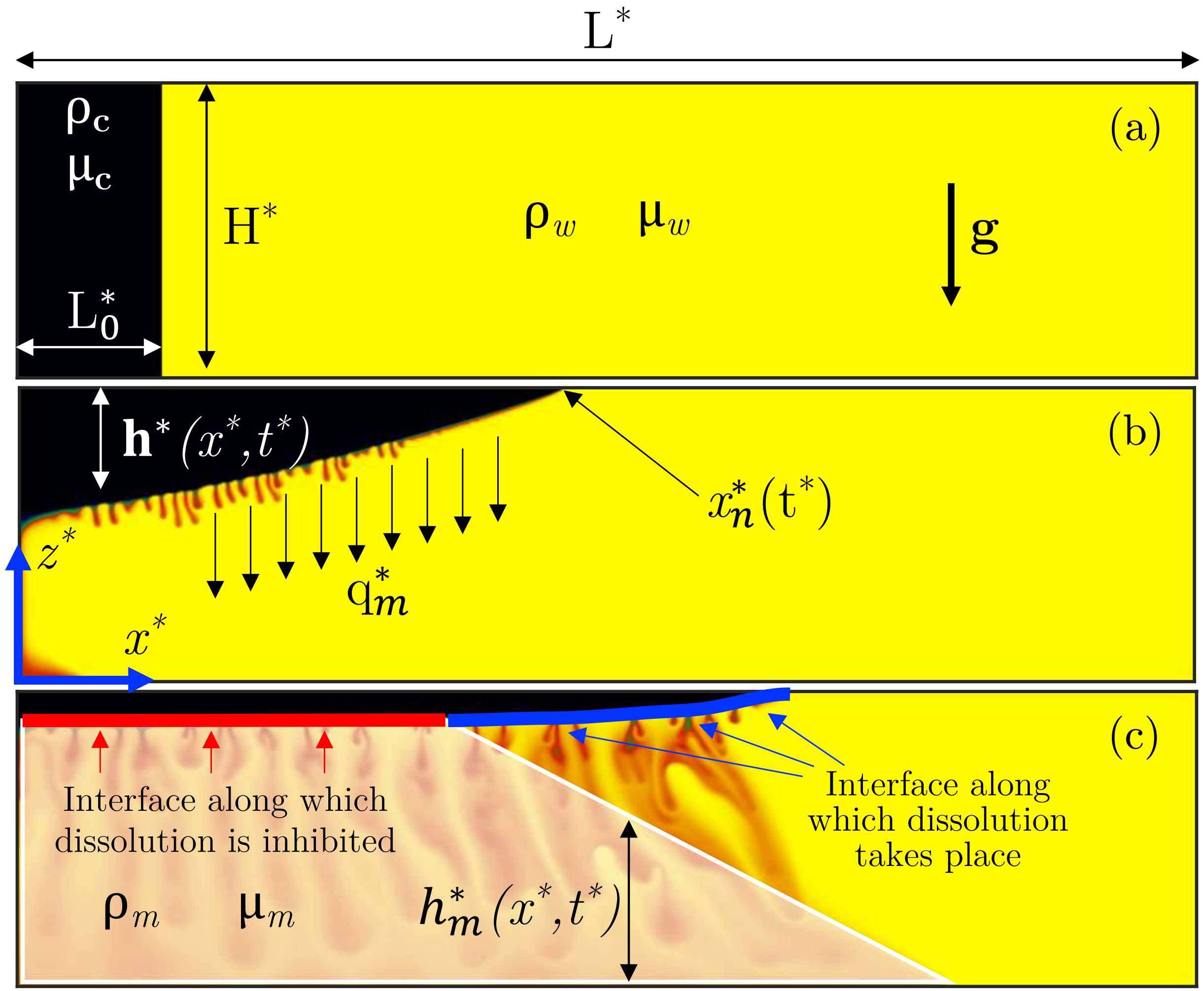


De Paoli, *Phys. Fluids.* (2021)

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

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

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



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

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

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

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

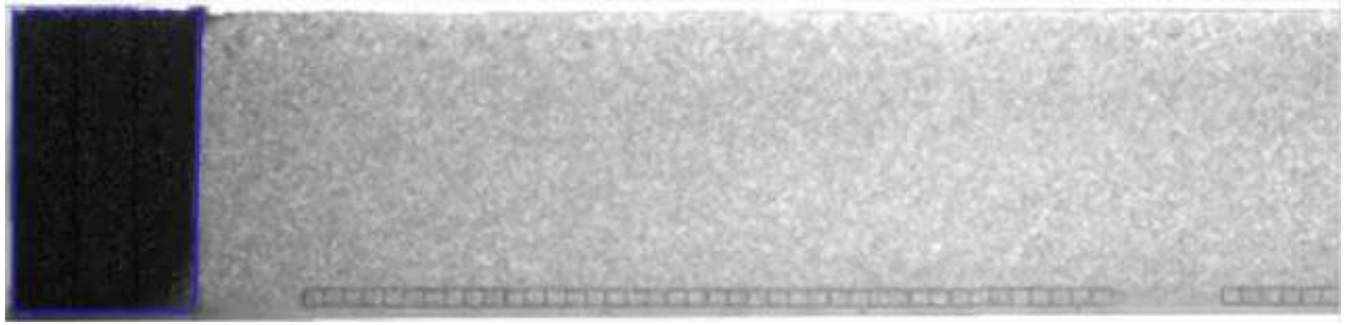
$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^*+1},$$

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 $X_v = \rho_m X_m/\rho_c$



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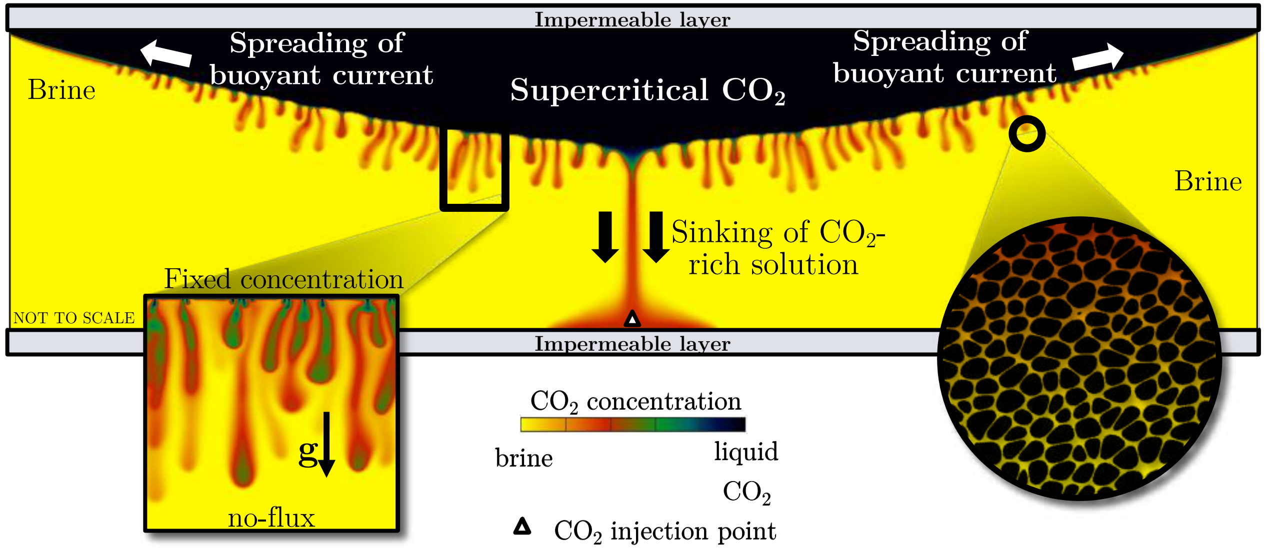

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$$f_m = \frac{M_m h_m^*/H^*}{(M-1)h^*/H^* + (M_m-1)h_m^*/H^* + 1},$$

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

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

How to determine the dissolution rate q_m^* ?

Dimensionless equations

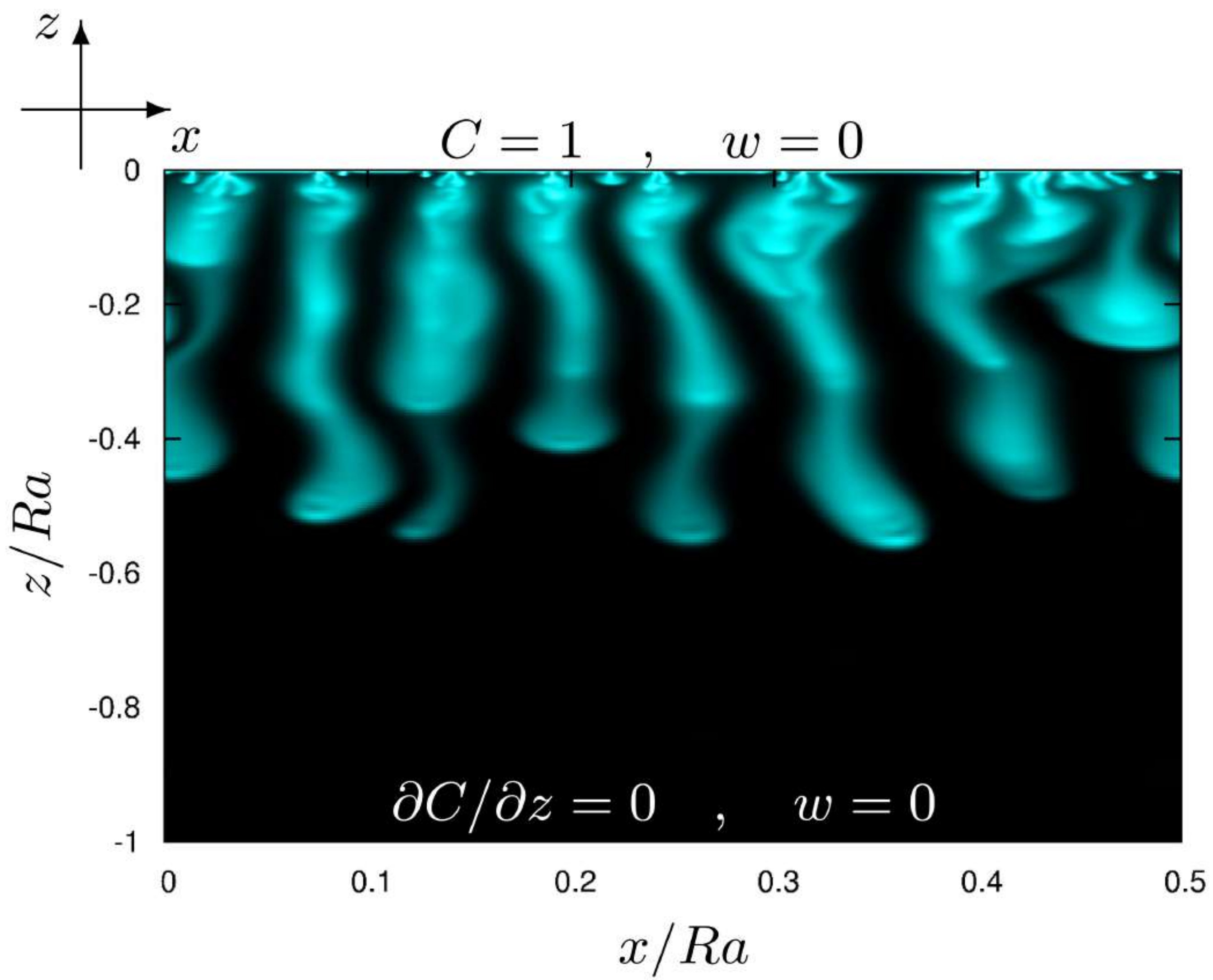
$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} = \frac{1}{Ra}\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial z^2}\right)$$

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

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

Governing parameter

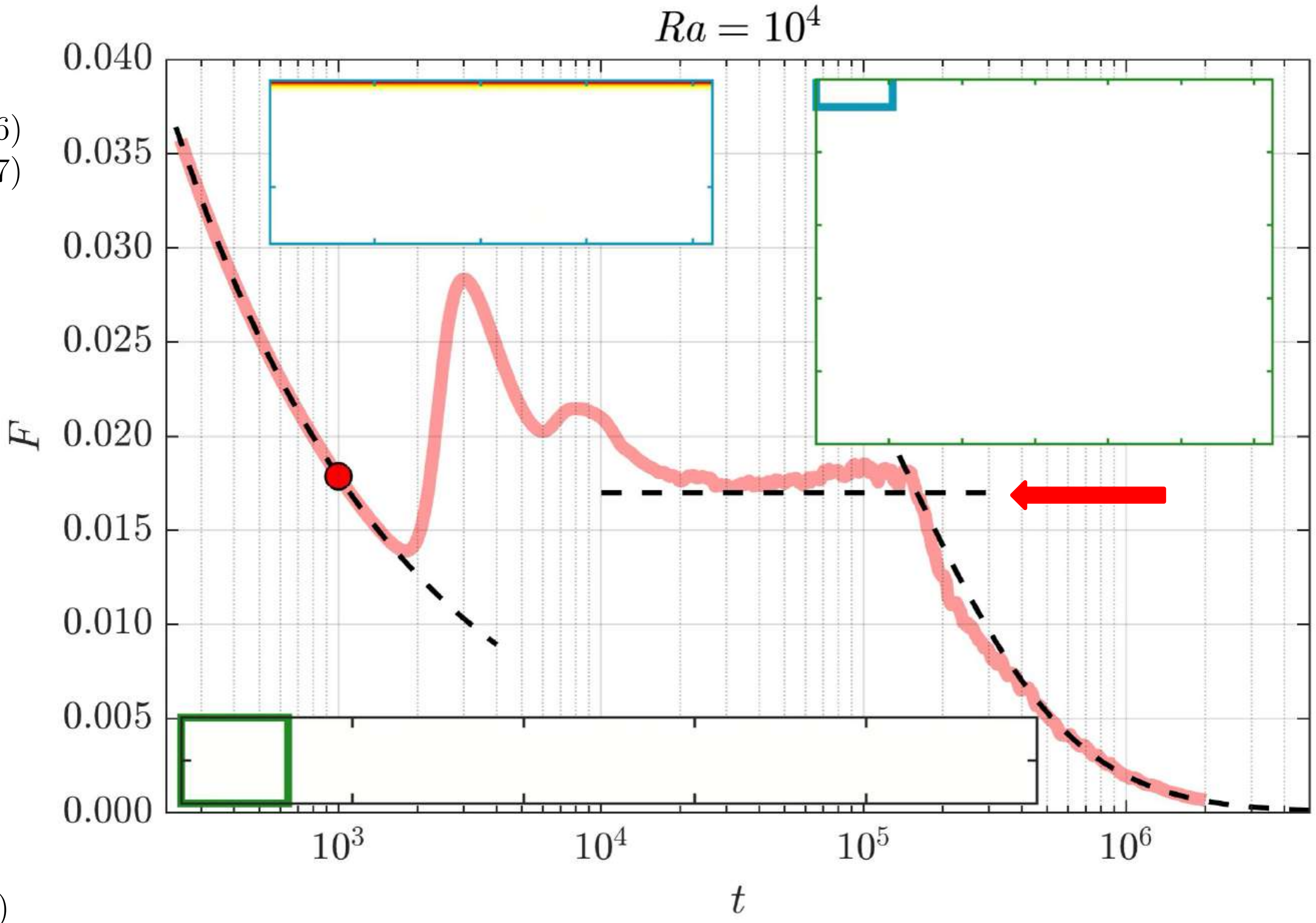
$$Ra = \frac{gH^* k_v \Delta\rho^*}{\mu \Phi D}$$



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

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

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



See also Slim, *J. Fluid Mech.* (2014)
Hewitt, Neufeld & Lister, *J. Fluid Mech.* (2013)

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

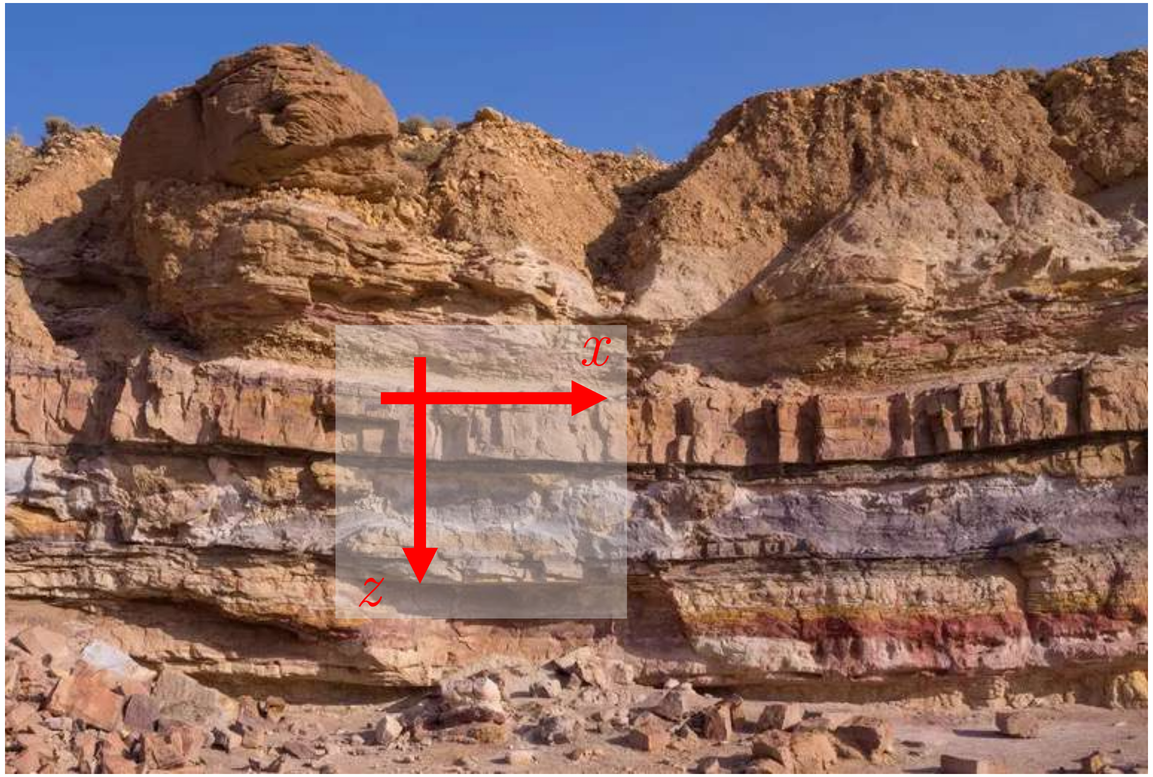
Problem formulation

Assumptions:
1. Homogeneous porous medium
2. Anisotropic porous medium
   - Principal directions of the permeability tensor aligned with the reference frame

https://www.intechopen.com/chapters/59029

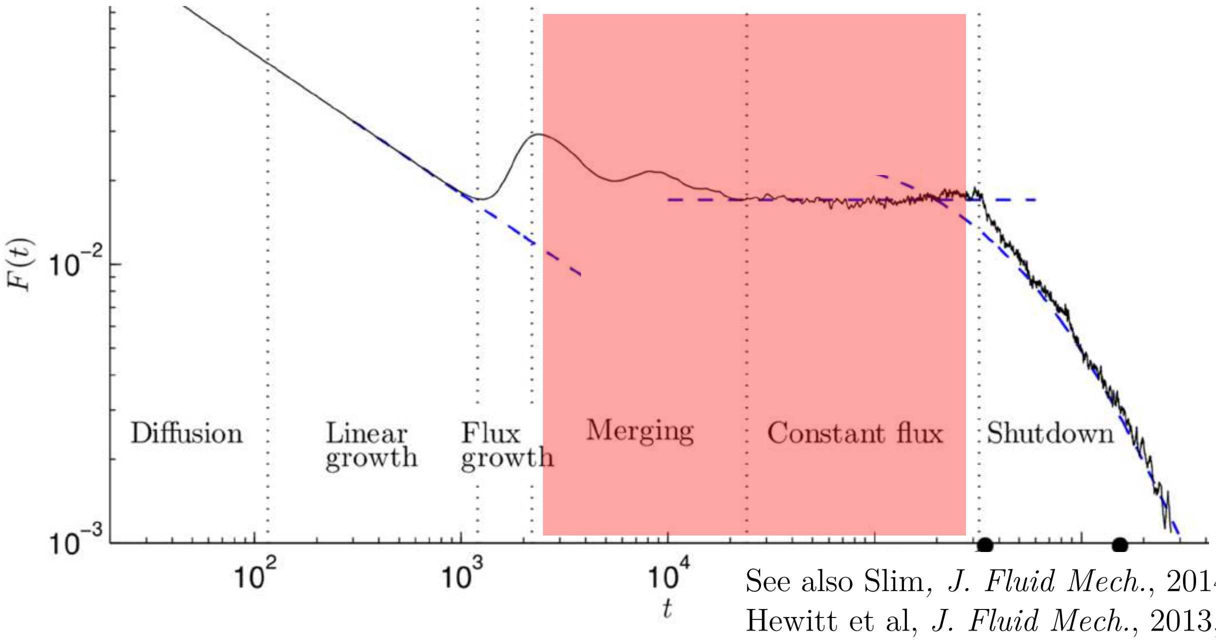
$$K = \begin{pmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{pmatrix}$$

$$K' = \begin{pmatrix} k'_{xx} & 0 & 0 \\ 0 & k'_{yy} & 0 \\ 0 & 0 & k'_{zz} \end{pmatrix}$$



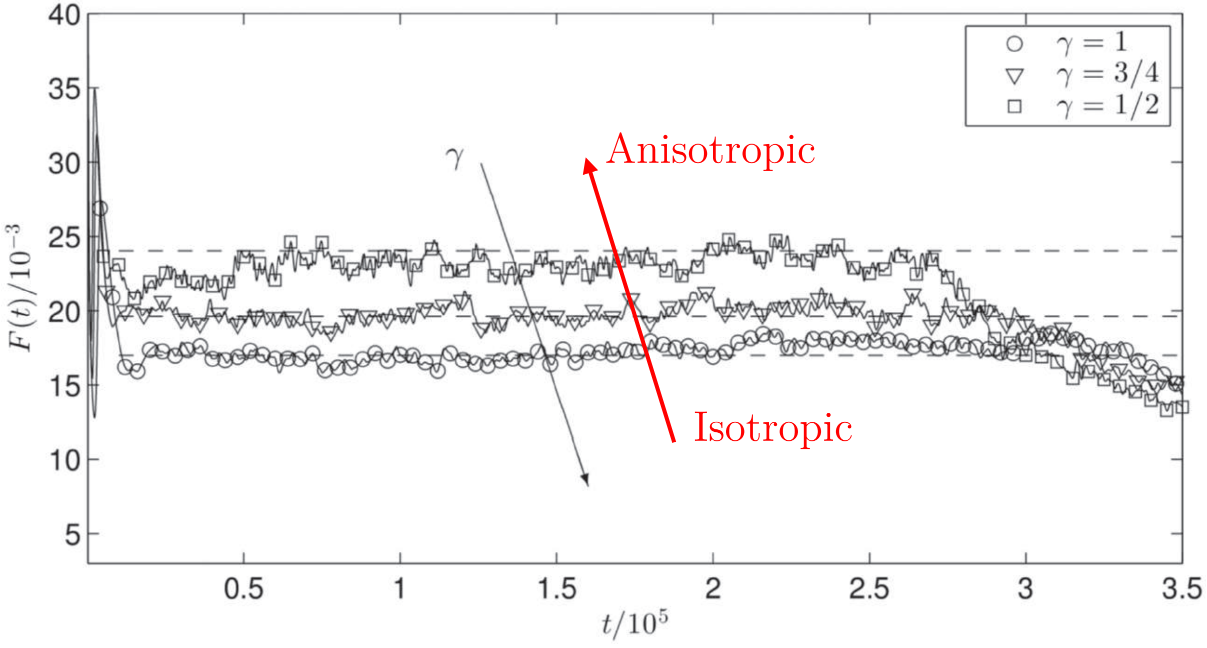
Rhododendrites/Wikimedia Commons/CC BY 4.0

isotropic medium



See also Slim, *J. Fluid Mech.*, 2014
Hewitt et al, *J. Fluid Mech.*, 2013,
De Paoli et al., *Phys. Fluids*, 2016, 2017

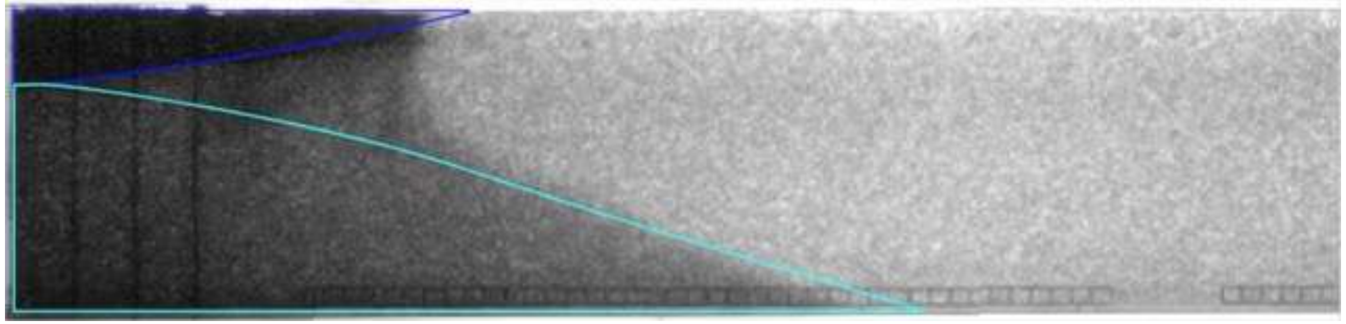
$$F(t) = \frac{1}{L}\int_0^L \frac{\partial C}{\partial z}\Big|_{z=0} dx$$



Convection-dominated $F(t) = 0.017$

Strong influence of γ on flux

$$q_m^{\ *} \equiv F(t) = 0.017\gamma^{-1/2}$$



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

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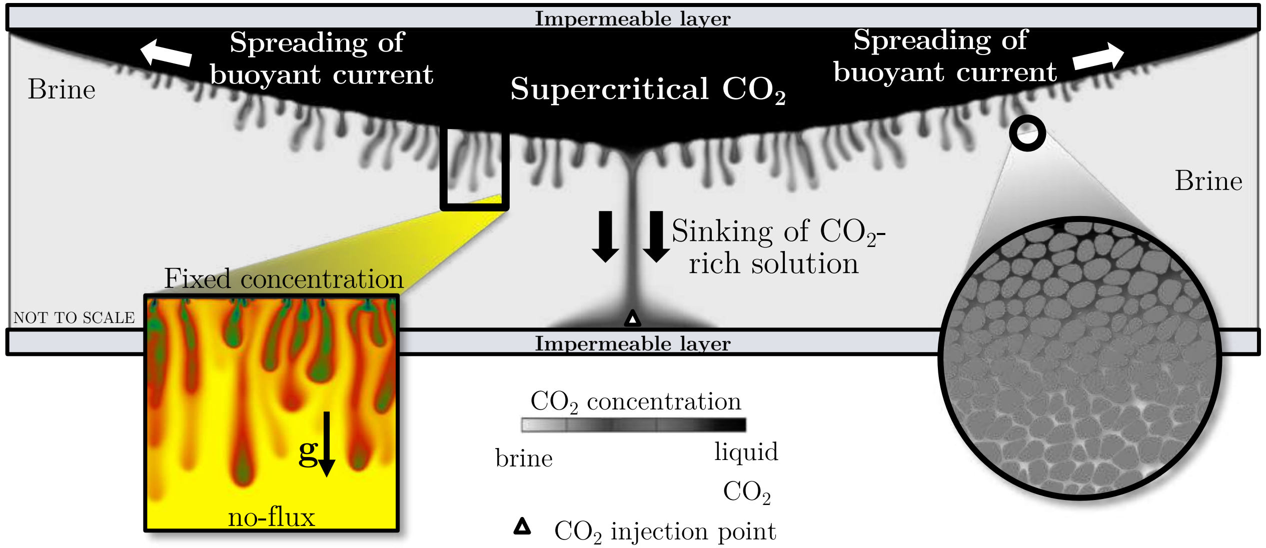
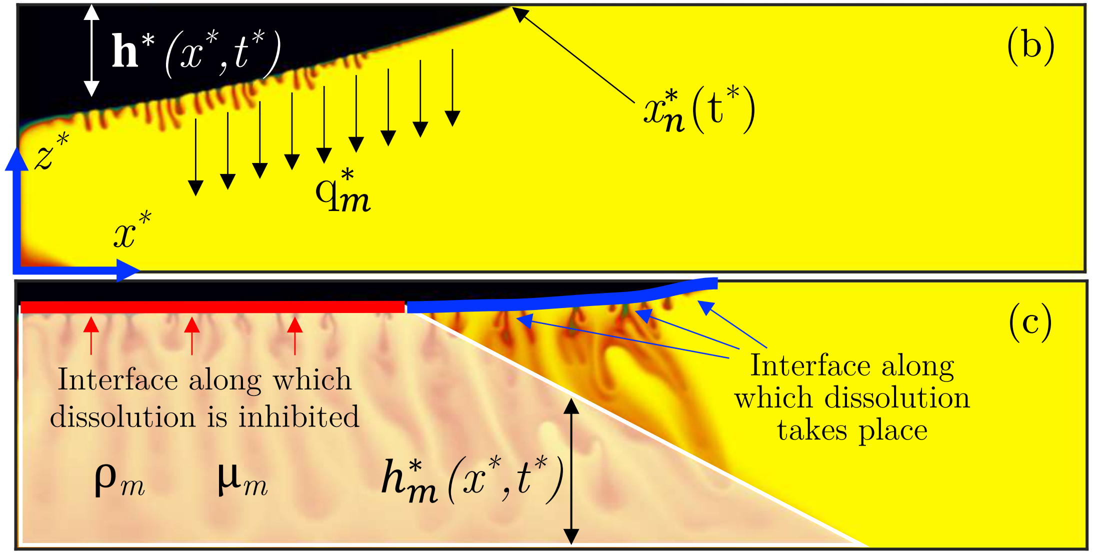


How to determine the dissolution rate q_m^* ?

Effect of anisotropy



Darcy-scale simulations:

⇩

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

⇩

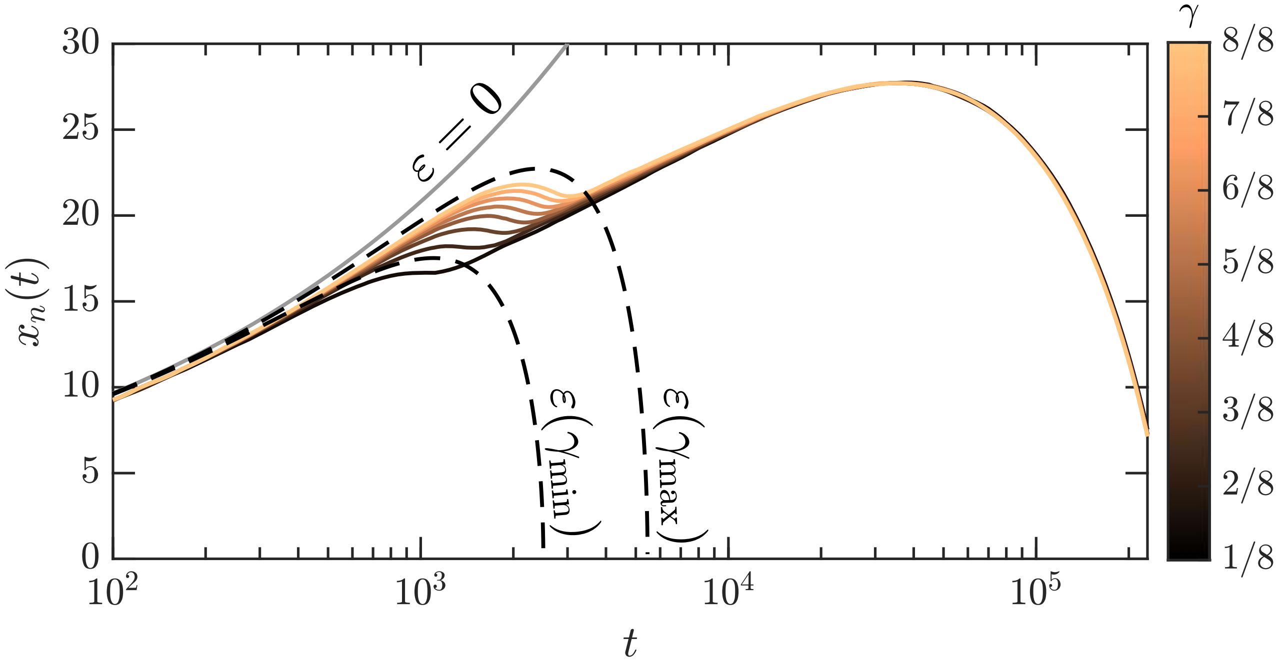
dissolution increases with the anisotropy of the medium

Sedimentary rocks are anisotropic

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

$\gamma = 1$ isotropic

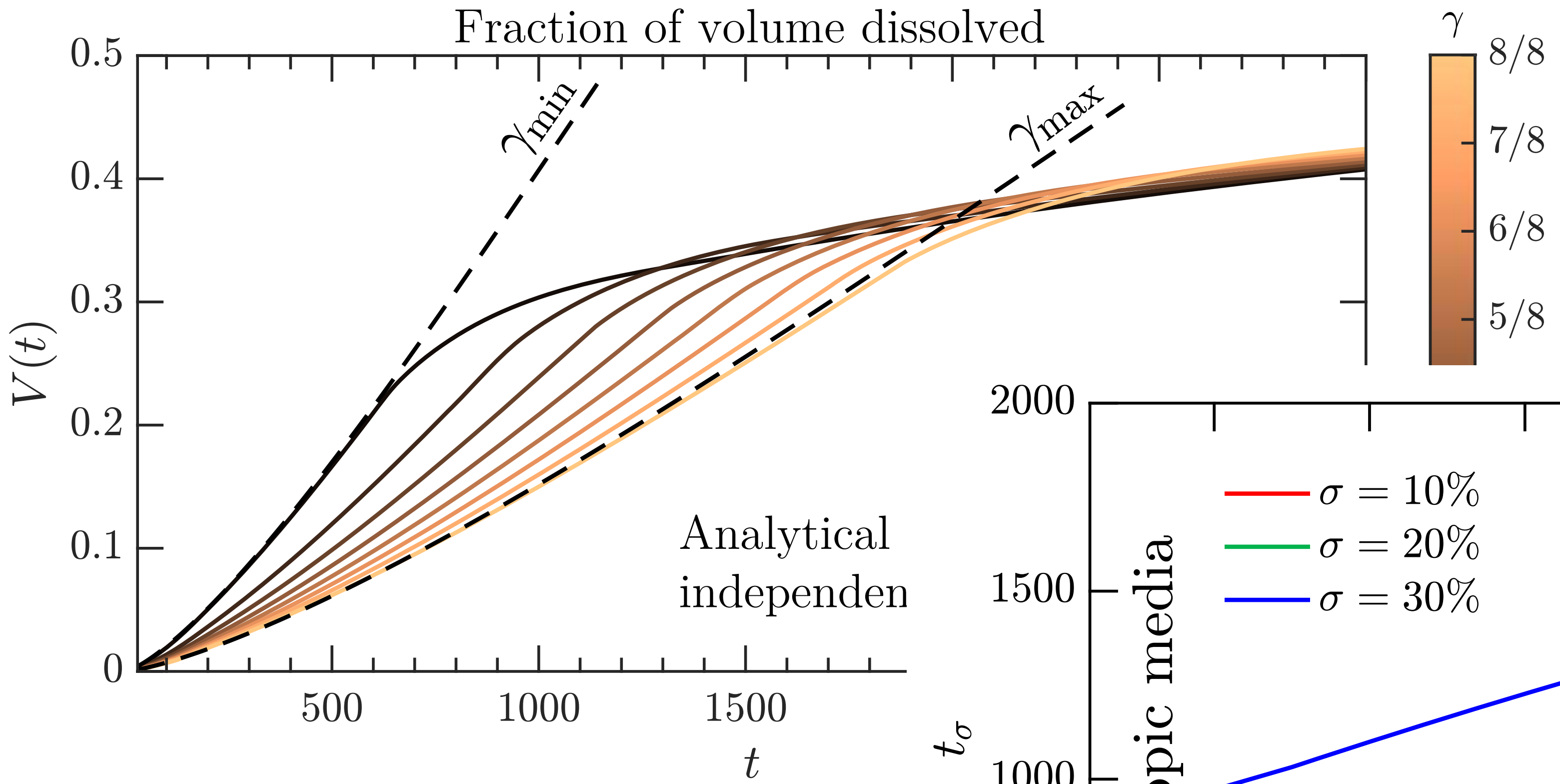
$\gamma = 1/8$ strongly anisotropic



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

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

Effect of anisotropy



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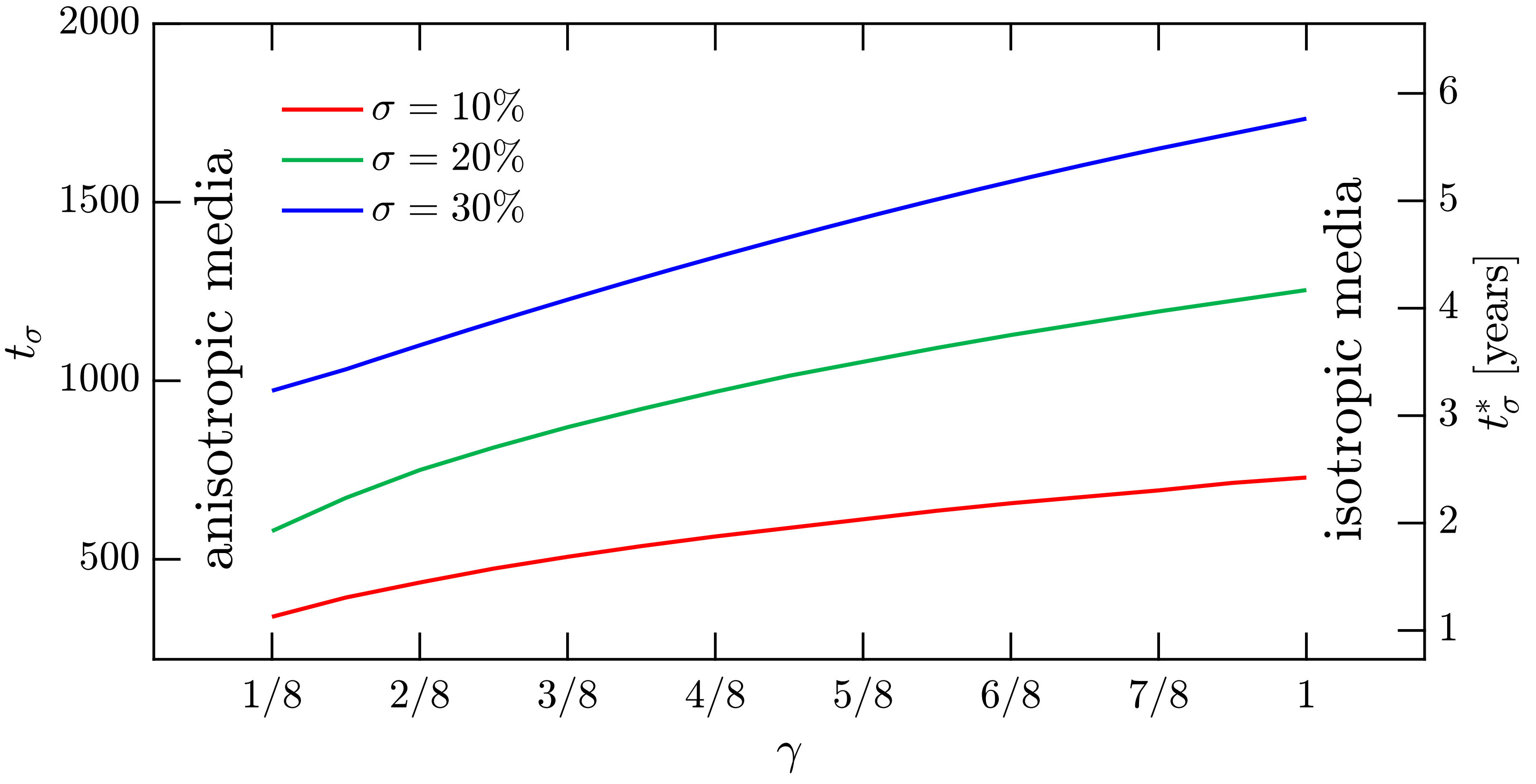
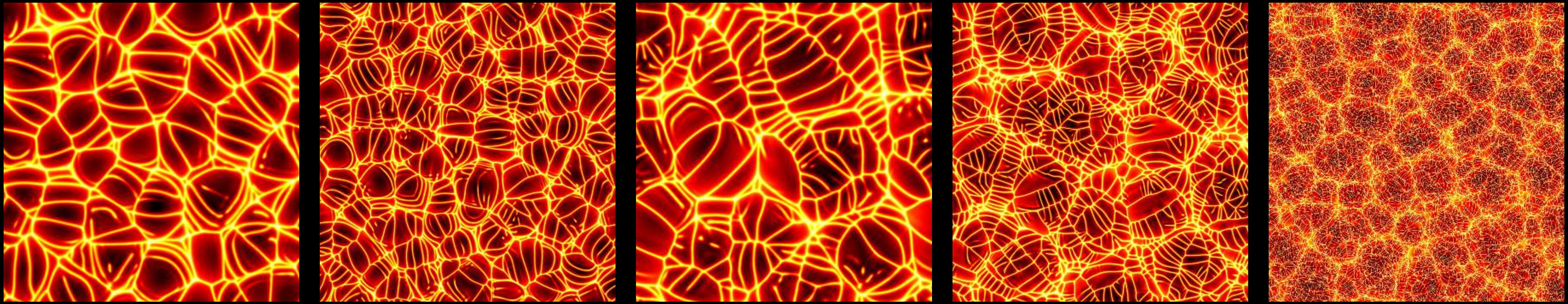


Long-term predictions
of real-scale reservoirs



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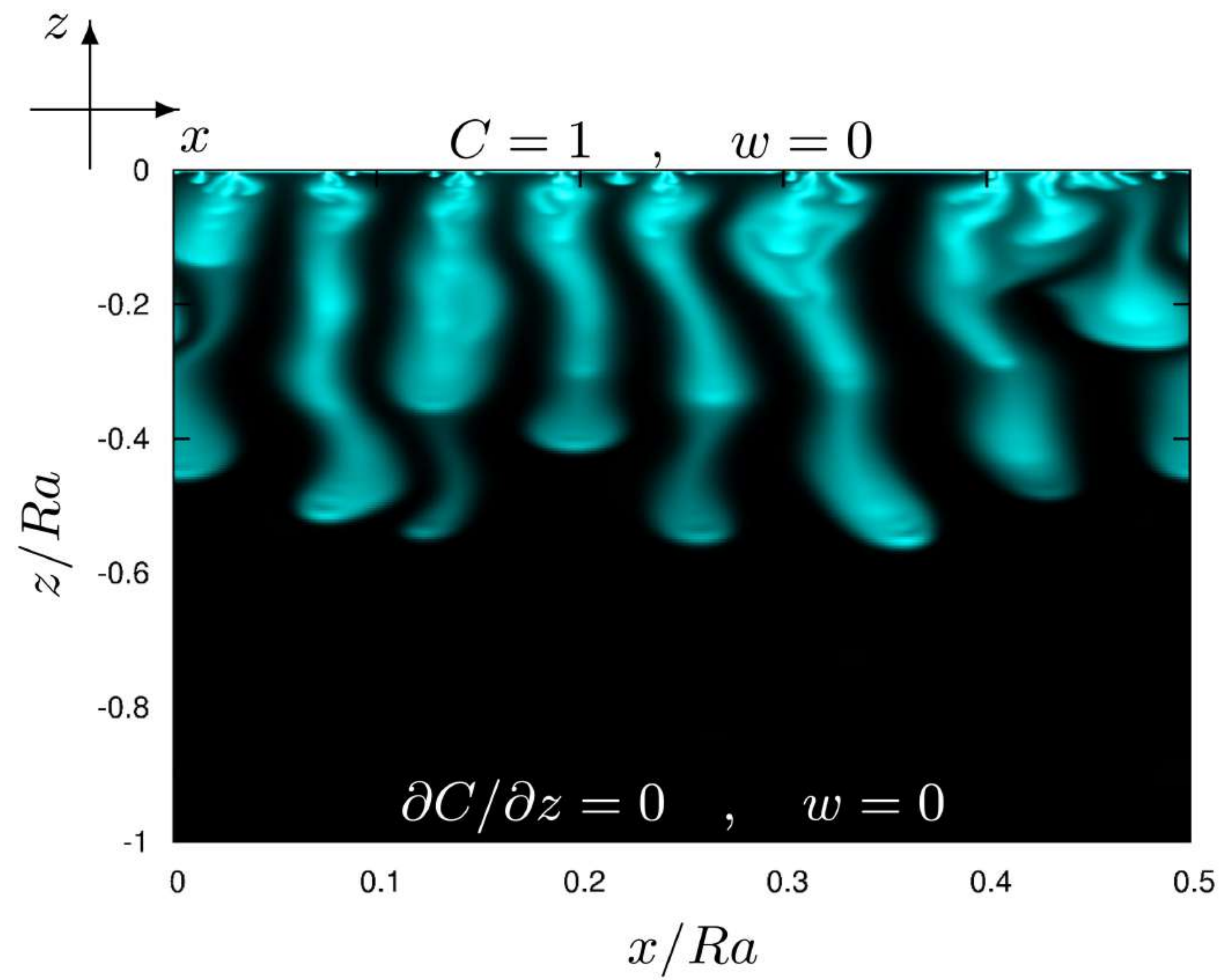
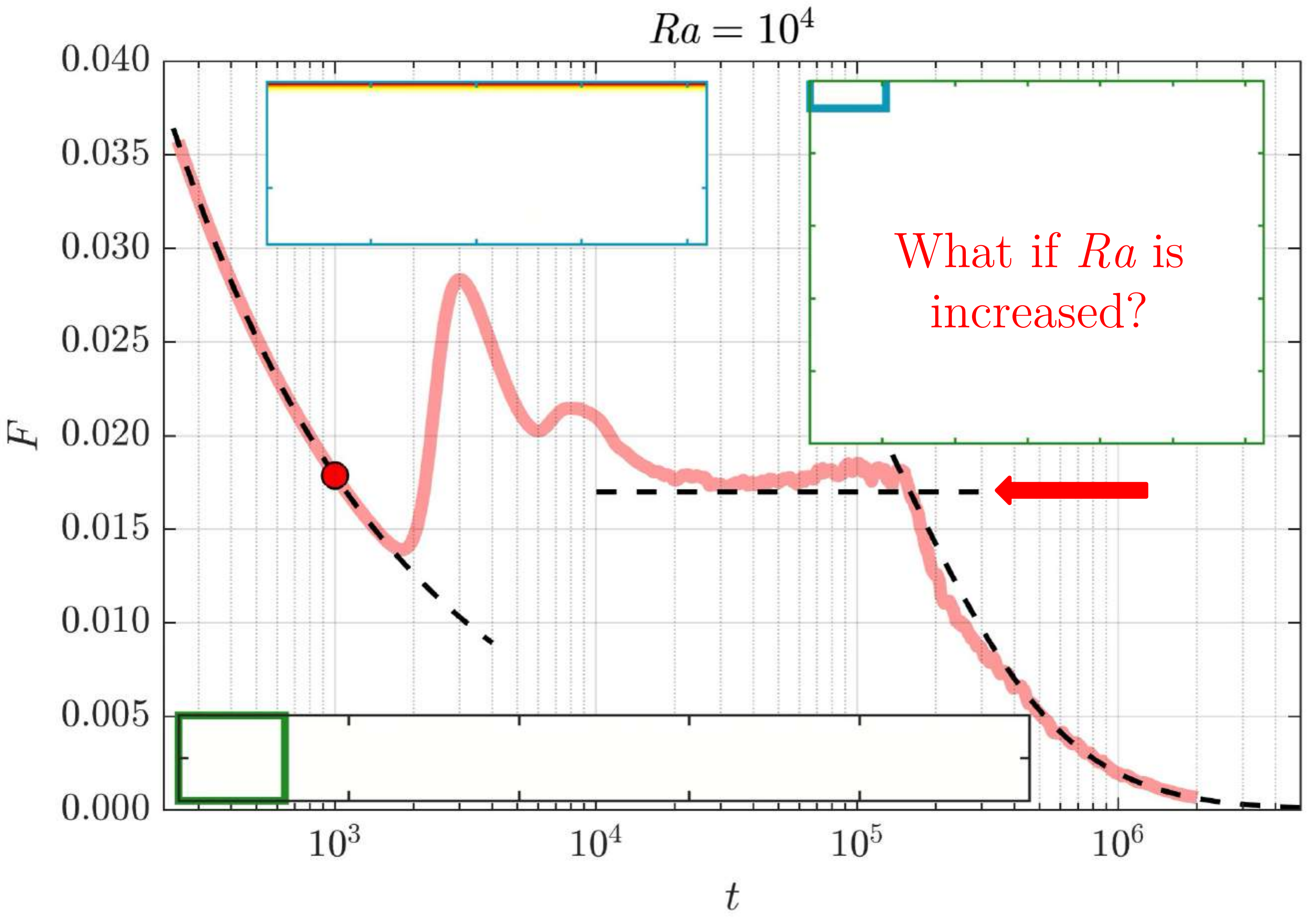


Convective dissolution process

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



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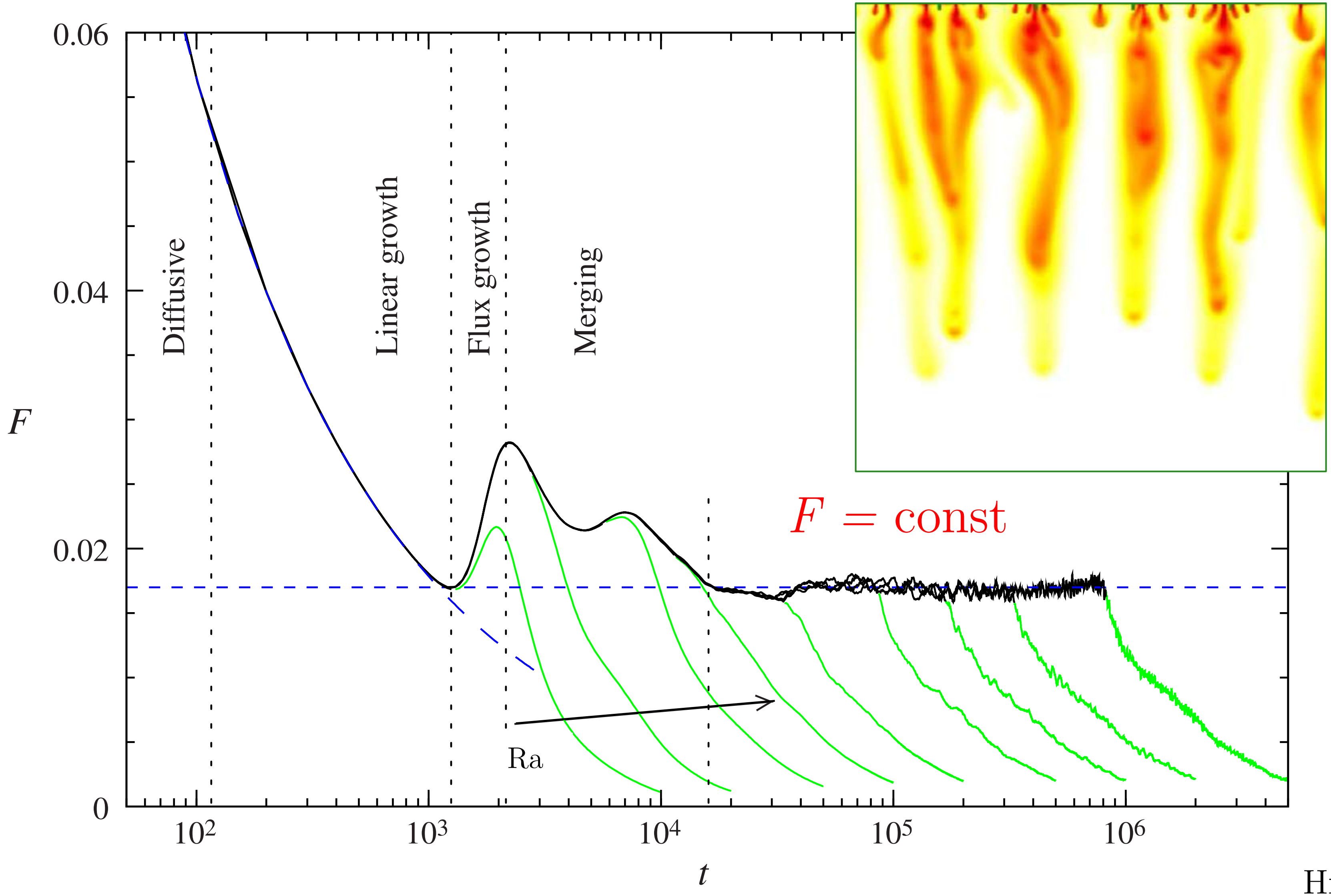
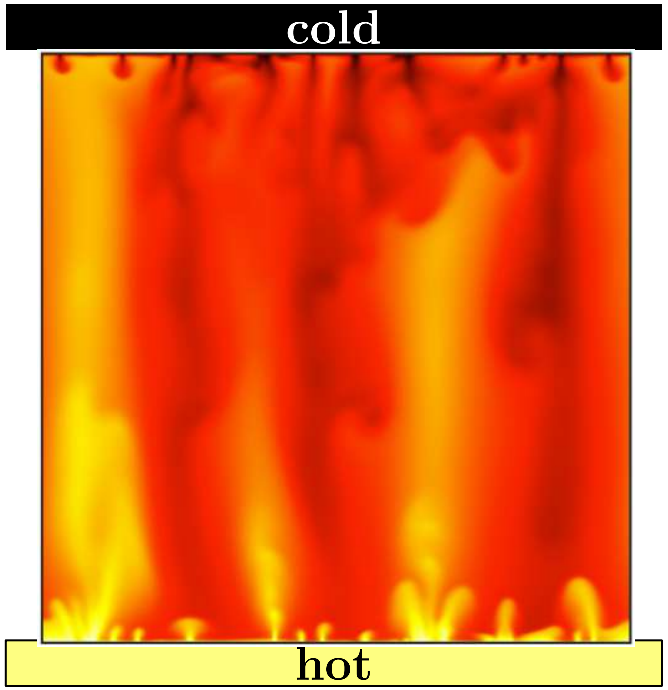
Convective dissolution process



Slim, *J. Fluid Mech.* (2014)

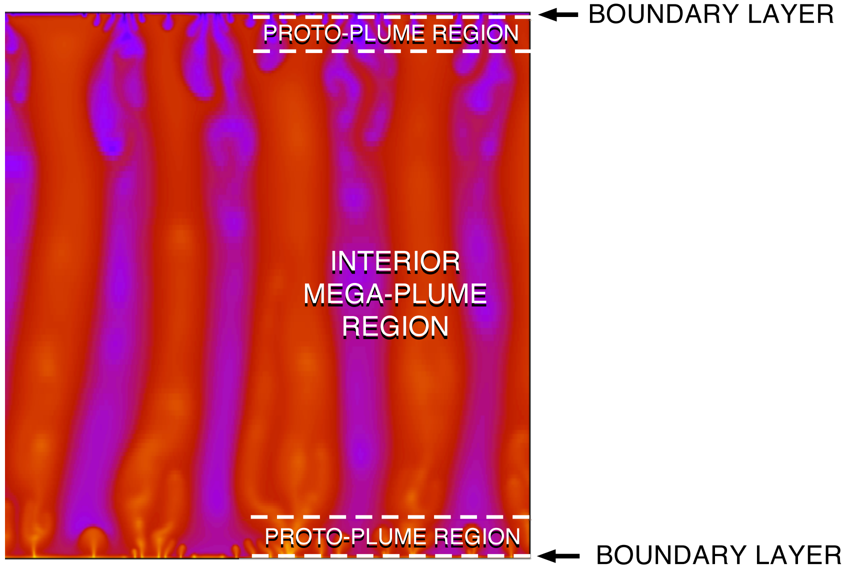
Exact closed energy budget



Hidalgo et al., *Phys. Rev. Lett.* (2012)
De Paoli, *arxiv* https://arxiv.org/abs/2310.01999

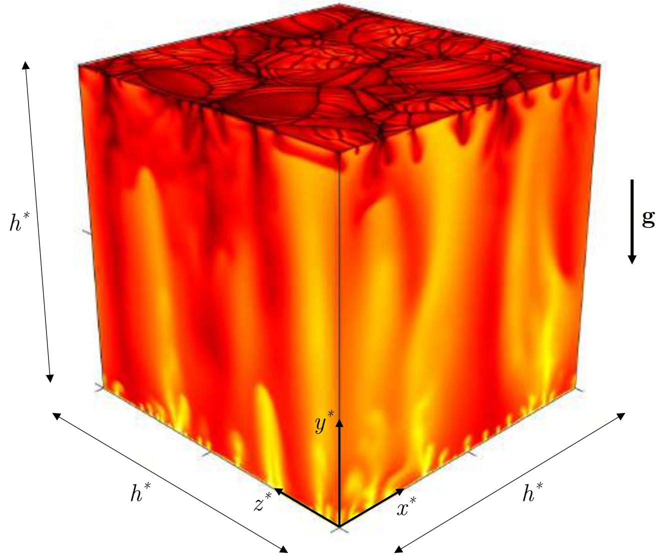
2D vs 3D convection

2D Darcy convection



Pau et al., *Adv. Water Res.* (2010)
Hidalgo et al., *Phys. Rev. Lett.* (2012)
Hewitt et al., *Phys. Rev. Lett.* (2012)
Hewitt et al., *J. Fluid Mech.* (2013)
Slim, *J. Fluid Mech.* (2014)
Wen et al. *J. Fluid Mech.* (2015)
De Paoli et al., *Phys. Fluids* (2016)
De Paoli et al., *Phys. Fluids* (2017)
Hewitt, *Proc. Royal Soc. A* (2020)
...

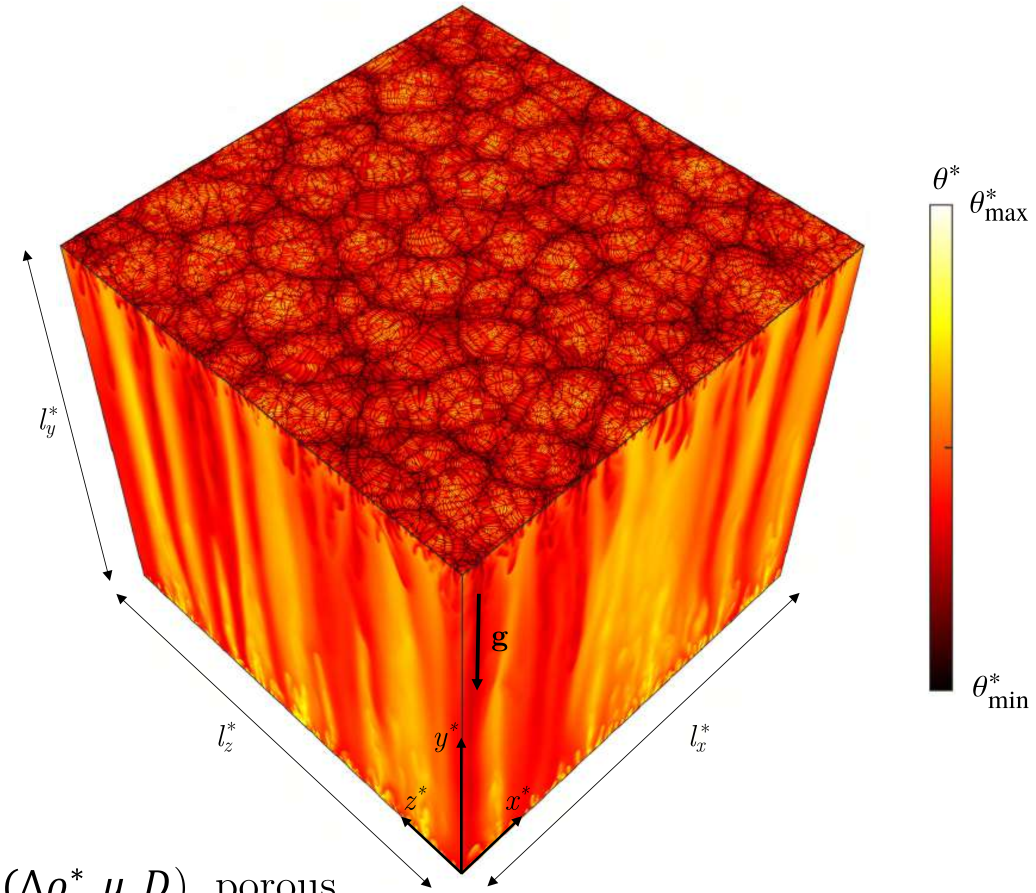
3D Darcy convection



Fu et al. Phil. Trans. Royal Soc. A (2013)
Hewitt et al., J. Fluid Mech. (2014)
Pirozzoli, De Paoli, Zonta & Soldati, J. Fluid Mech. (2021)
De Paoli, Pirozzoli, Zonta & Soldati, J. Fluid Mech. (2022)

3D convection little explored compared to the 2D case due to huge computational costs

Methodology



Fluid $(\Delta\rho^*, \mu, D)$, porous medium (κ, ϕ) and domain (l_y^*) properties → $Ra = g\Delta\rho^*\kappa l_y^*/(\phi D\mu)$

Pirozzoli, De Paoli, Zonta & Soldati, *J. Fluid Mech.* (2021)
De Paoli, Pirozzoli, Zonta & Soldati, *J. Fluid Mech.* (2022)

See also Hewitt, Neufeld & Lister, *J. Fluid Mech.* (2014)

Equations

$$\frac{\partial\theta}{\partial t} + \nabla\cdot\left(\mathbf{u}\theta - \frac{1}{\mathrm{Ra}}\nabla\theta\right) = 0,$$

$$\nabla\cdot\mathbf{u} = 0 \quad , \quad \mathbf{u} = -\left(\nabla p - \theta\mathbf{j}\right),$$

Boundary conditions

$$v(y=0) = 0 \quad , \quad \theta(y=0) = 1,$$
$$v(y=1) = 0 \quad , \quad \theta(y=1) = 0.$$

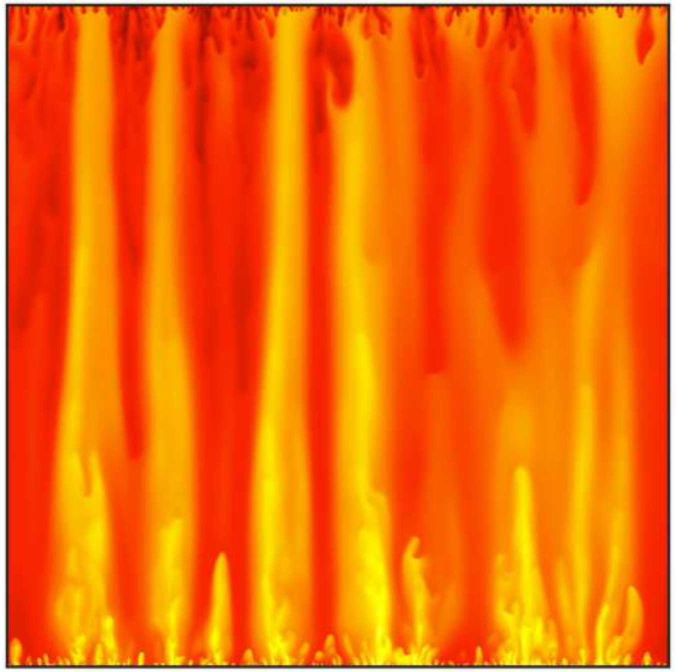
Note that the temperature field has replaced the concentration field in this formulation

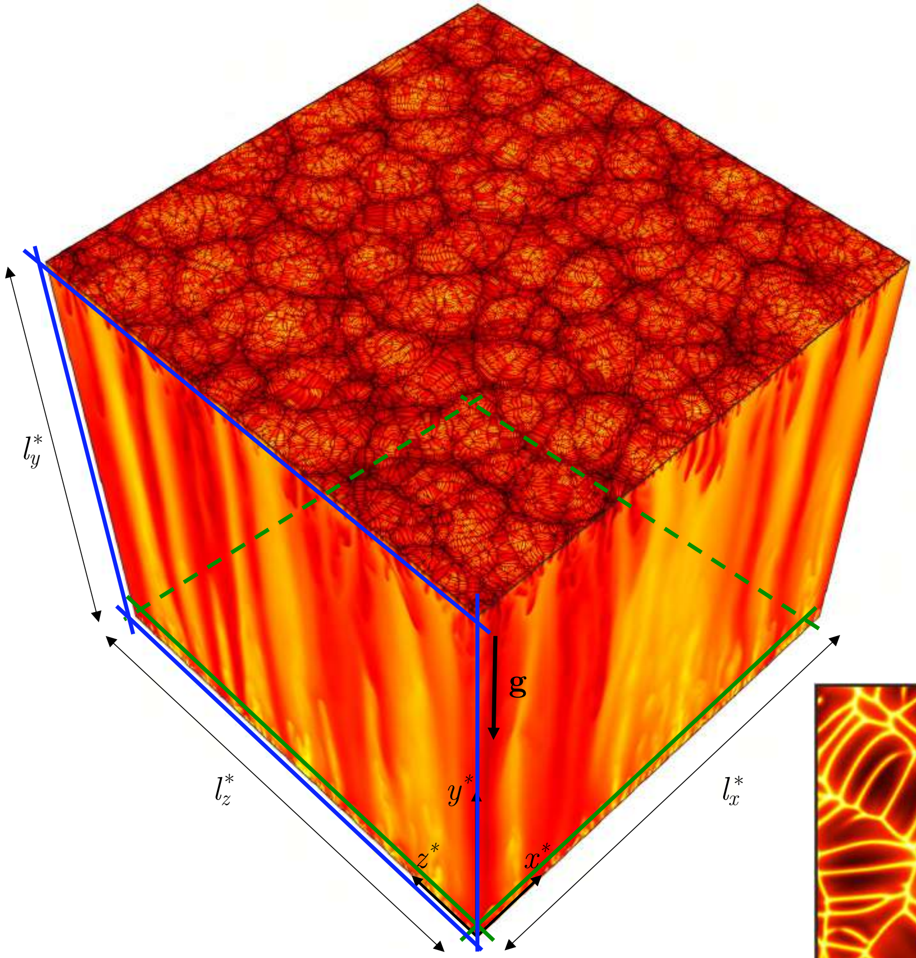
Simulations performed

Simulation	Ra	$l_x/l_y \times l_z/l_y$	$N_x \times N_z \times N_y$
Ra_1	1.0×10^3	4×4	$384\times384\times32$
Ra_2	2.5×10^3	4×4	$768\times768\times64$
Ra_5	5.0×10^3	4×4	$1536\times1536\times128$
Ra_7	7.5×10^3	4×4	$2304\times2304\times192$
Ra_{10}	1×10^4	1×1	$768\times768\times256$
Ra_{20}	2×10^4	1×1	$1536\times1536\times512$
Ra_{30}	3×10^4	1×1	$2304\times2304\times768$
Ra_{40}	4×10^4	1×1	$3072\times3072\times1024$
Ra_{80}	8×10^4	1×1	$6144\times6144\times2048$

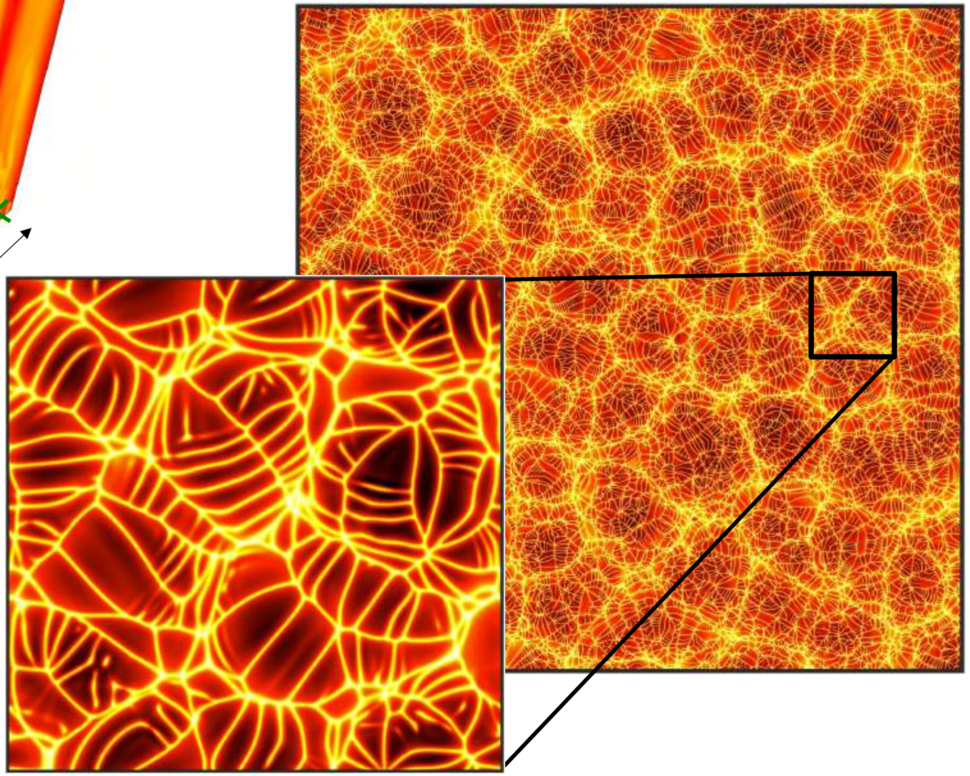
$\mathrm{Ra} = 8 \times 10^4$

y-z slice ($x = 0$)





x-z slice ($y = 0.01$)



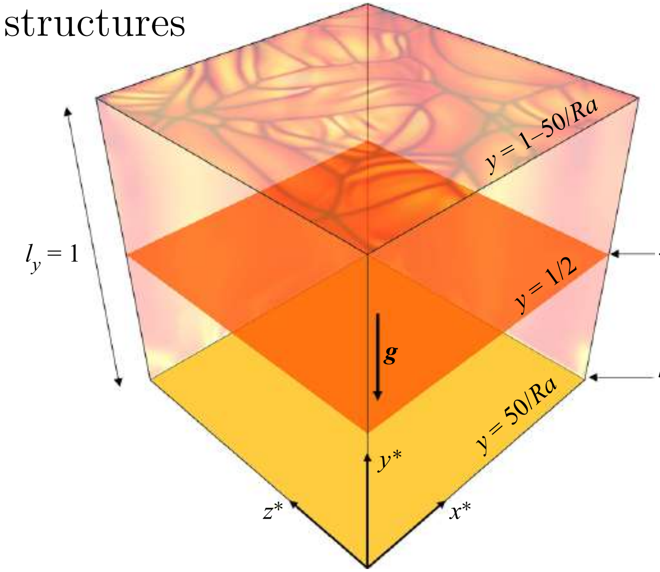
Pirozzoli, De Paoli, Zonta & Soldati, *J. Fluid Mech* (2021)

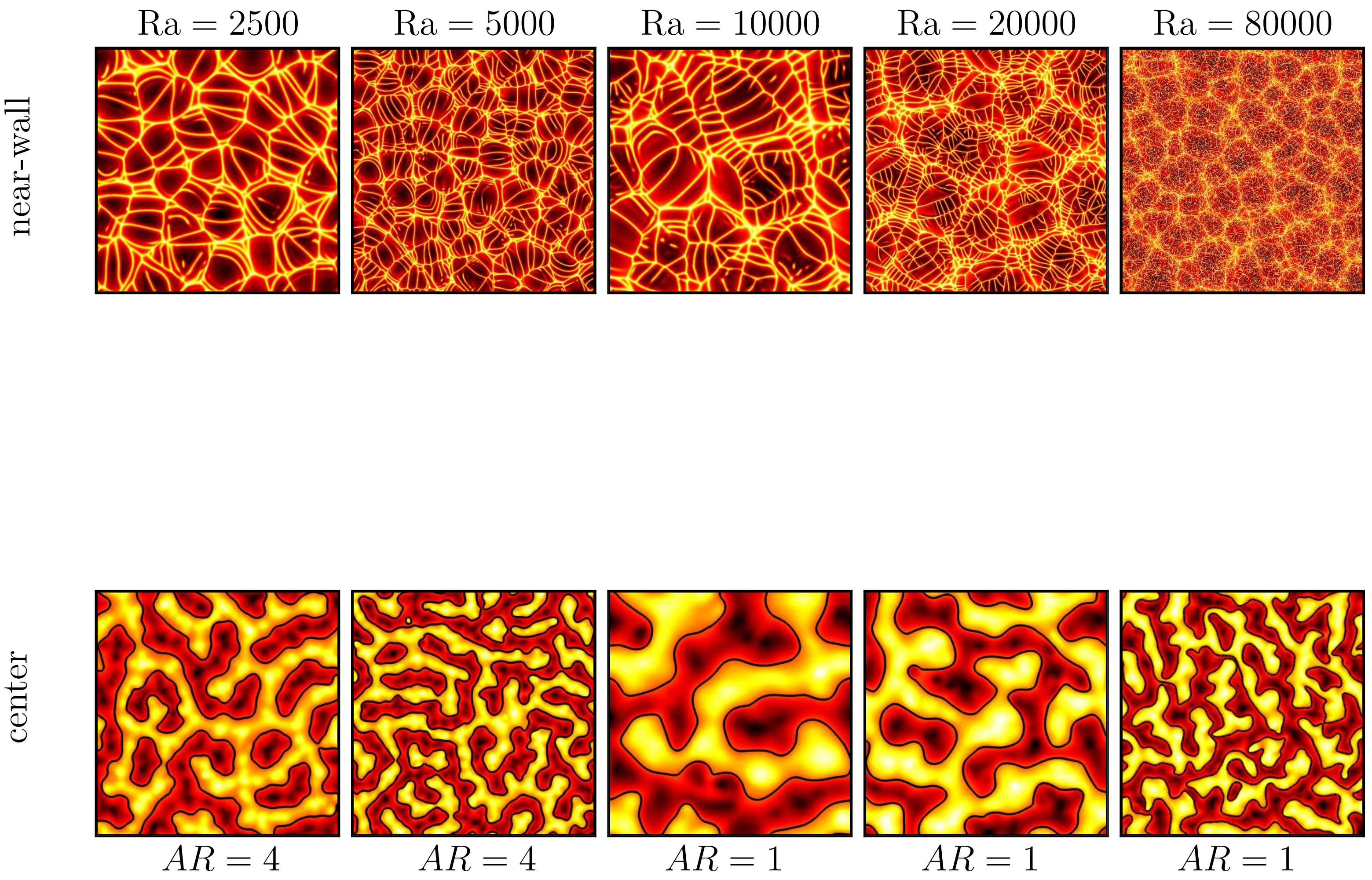
Supercells and megaplumes

Mean radial wave number

$$\overline{k}_r(y) = \left\langle \frac{\int\int \sqrt{k_x^2 + k_z^2}\, E(k_x, k_z)\, \mathrm{d}x\mathrm{d}z}{\int\int E(k_x, k_z)\, \mathrm{d}x\mathrm{d}z} \right\rangle$$

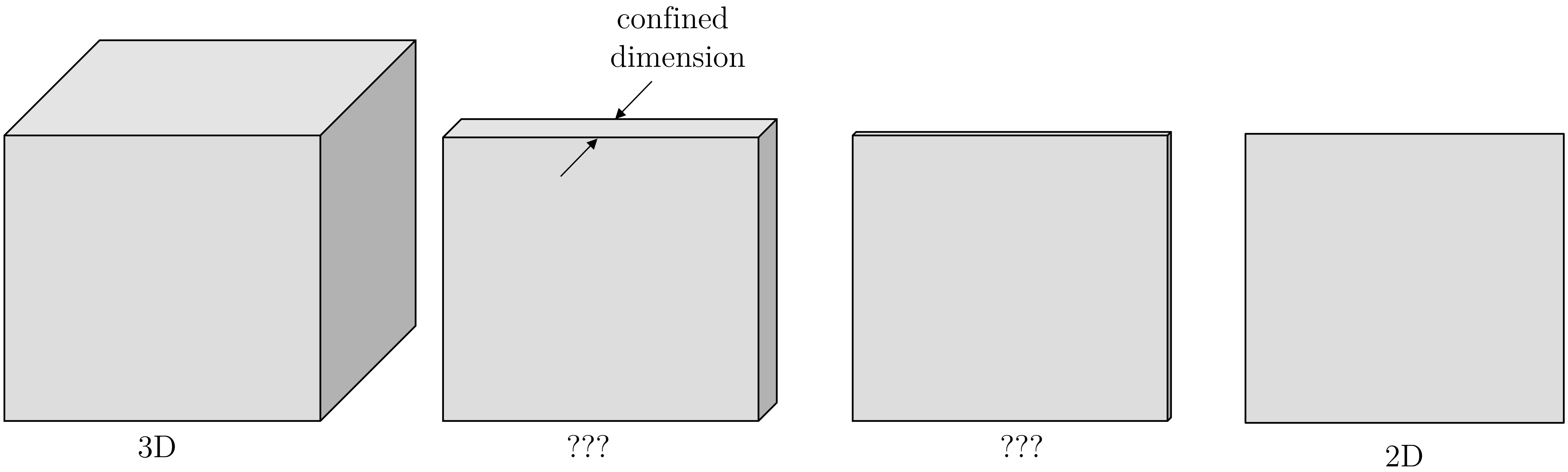
Following Krug *et al.*, *J. Fluid Mech.* (2018), we filter out the small-scale structures





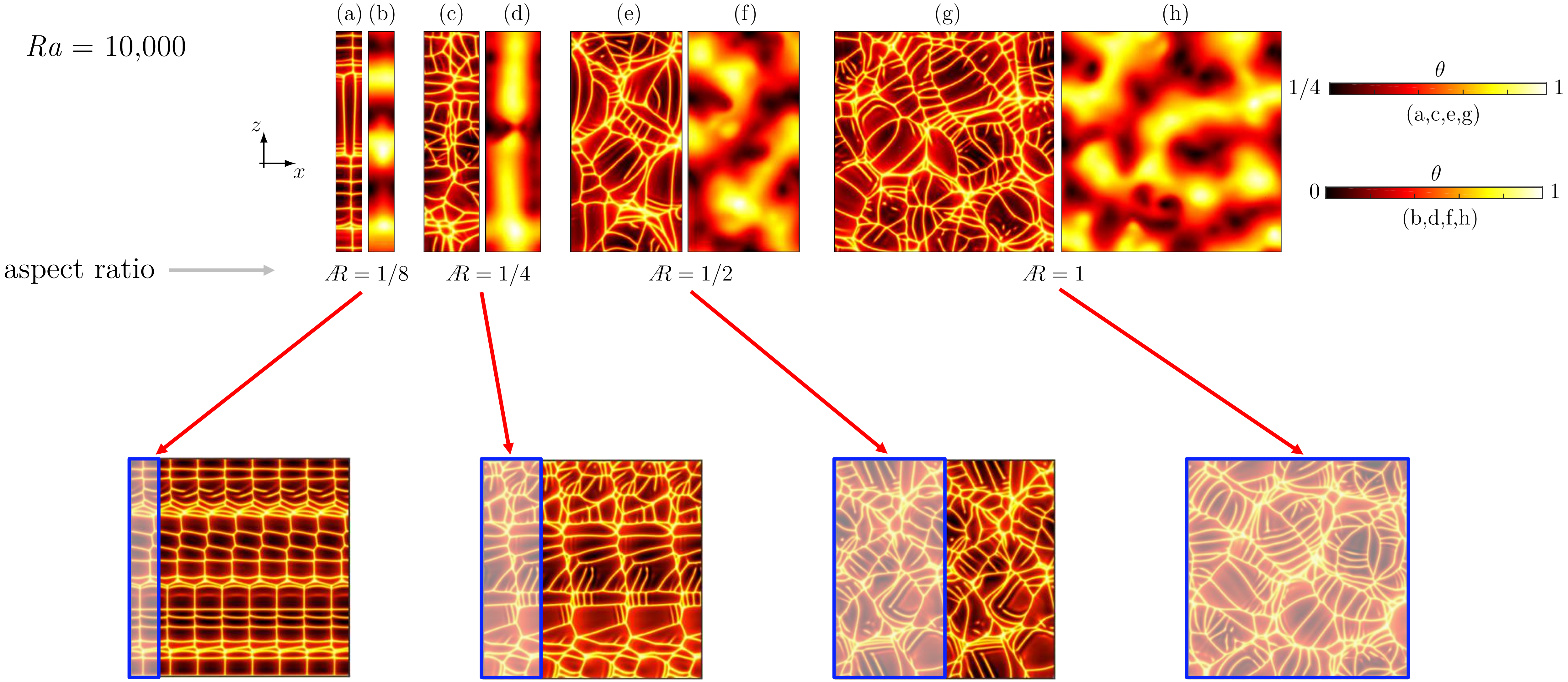
Supercells are the footprint of megaplumes

Dimensional transition



De Paoli https://arxiv.org/abs/2310.01999
Boffetta and Borgnino, *Phil. Trans. R. Soc. A* (2021)
Borgnino *et al.*, *Phys. Rev. Fluids* (2021)

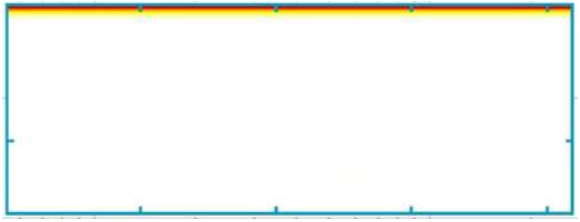
Assessment of domain size effects



Pirozzoli, De Paoli, Zonta & Soldati, *J. Fluid Mech.* (2021)
De Paoli, Pirozzoli, Zonta & Soldati, *J. Fluid Mech.* (2022)

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)



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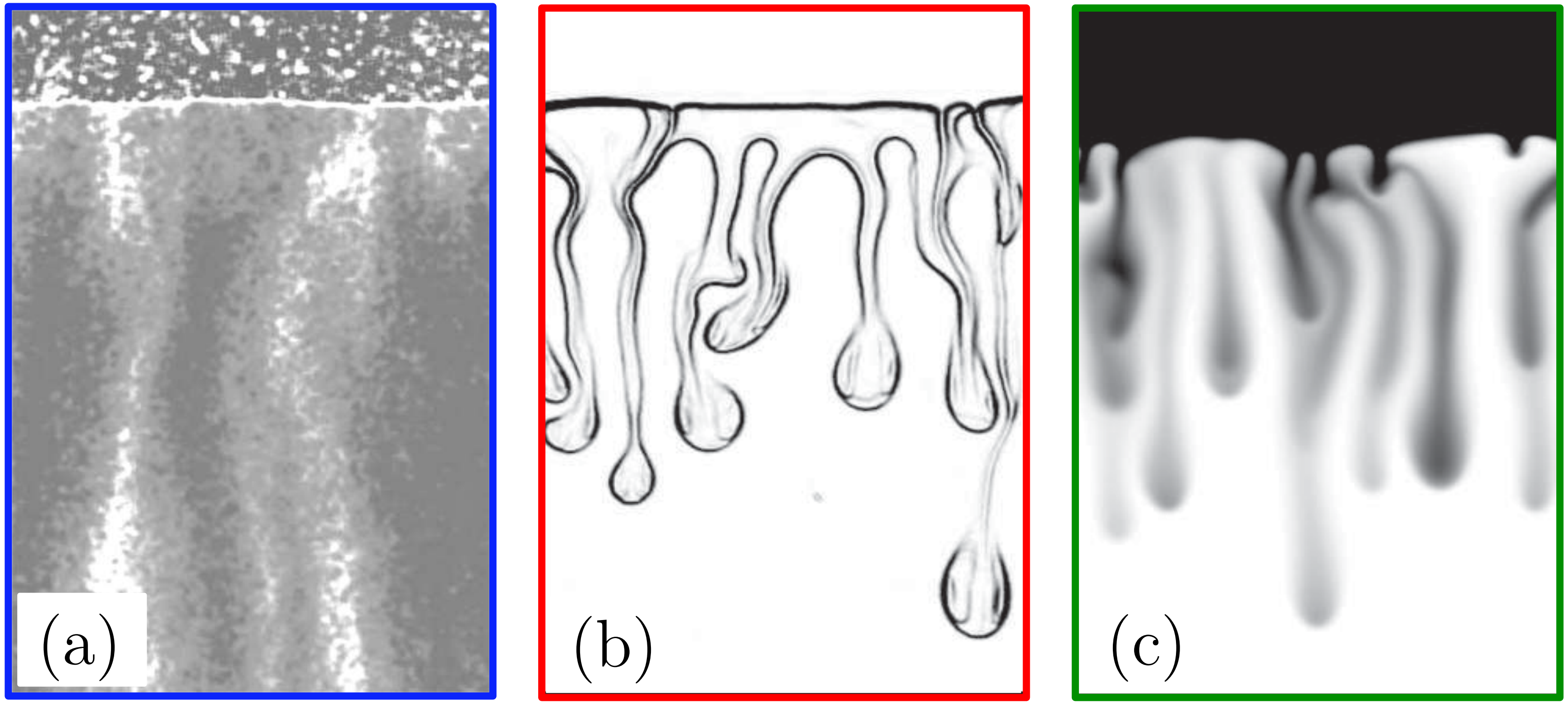
Darcy simulations: $\mathrm{Sh} \sim \mathrm{Ra}$ (Hidalgo et al., *Phys. Rev. Lett.* 2012)



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

See De Paoli https://arxiv.org/abs/2310.01999 for a detailed discussion

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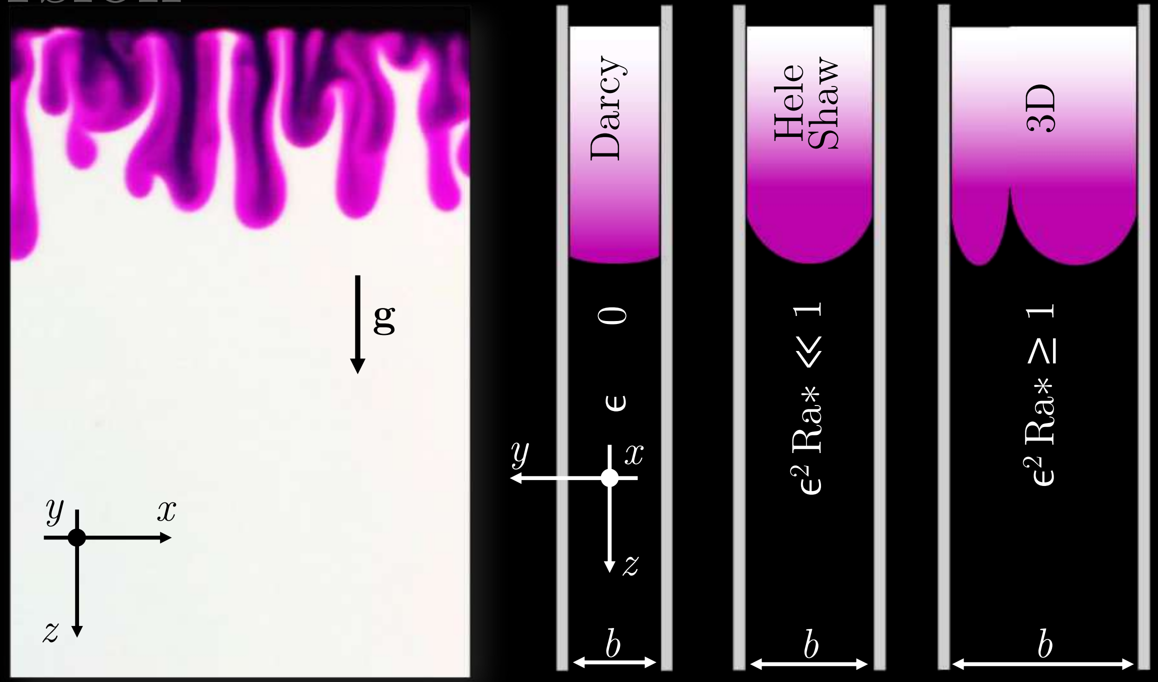

front view

side views

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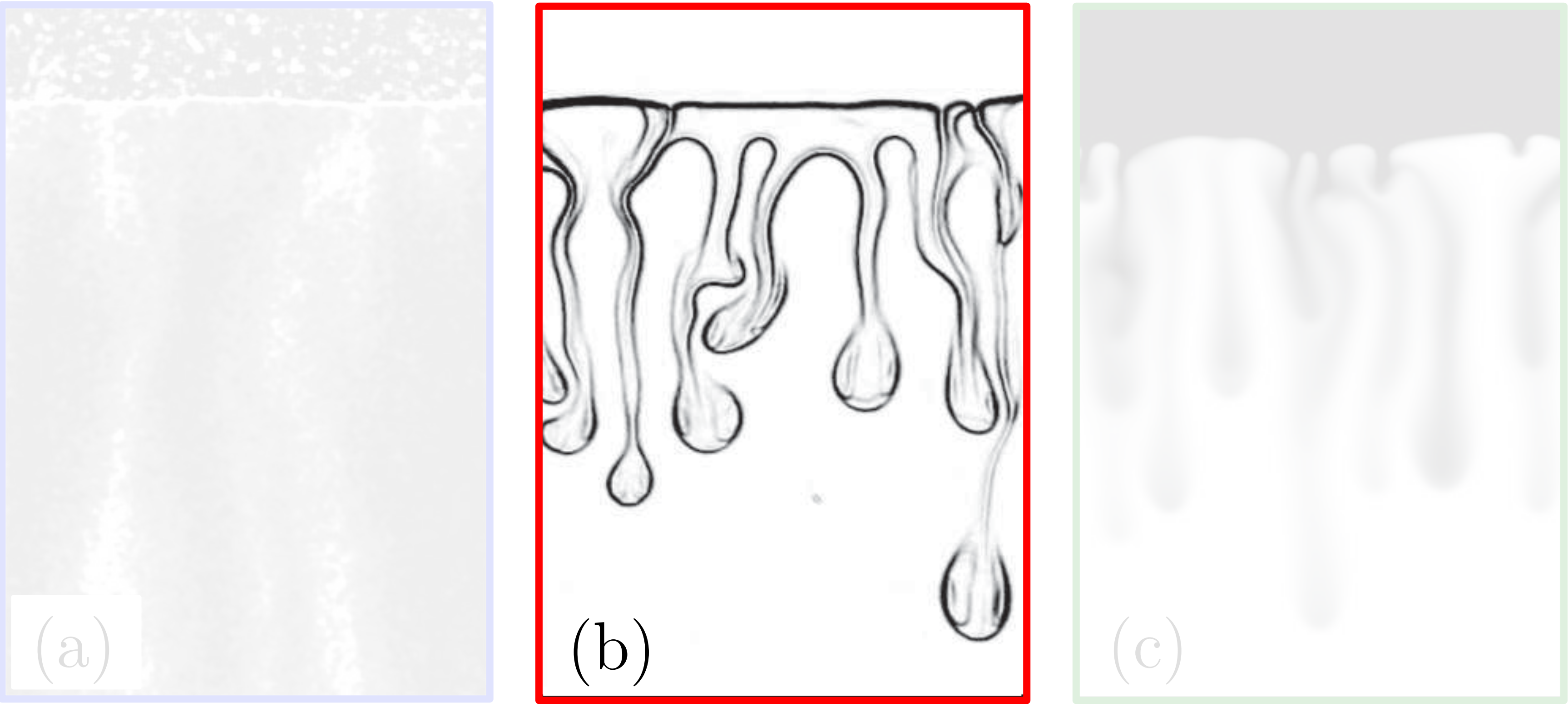

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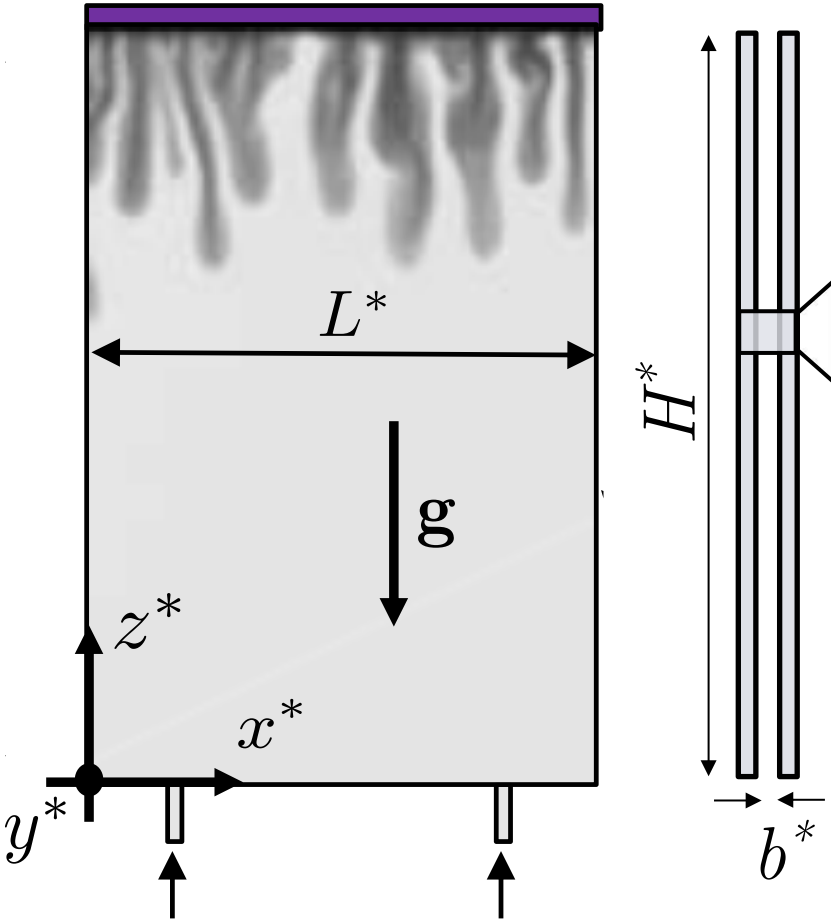
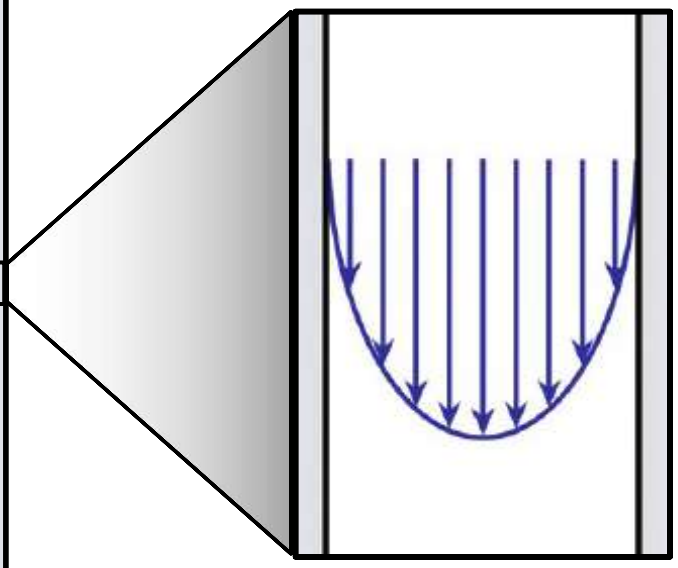
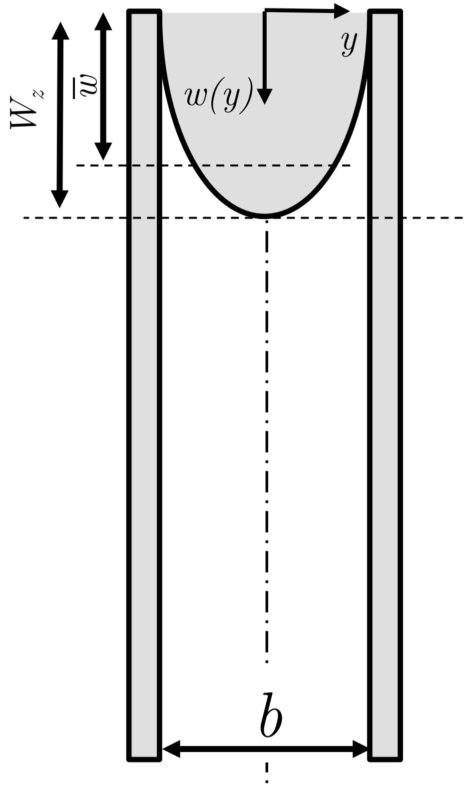
Experiments in Hele-Shaw cells





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



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

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

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

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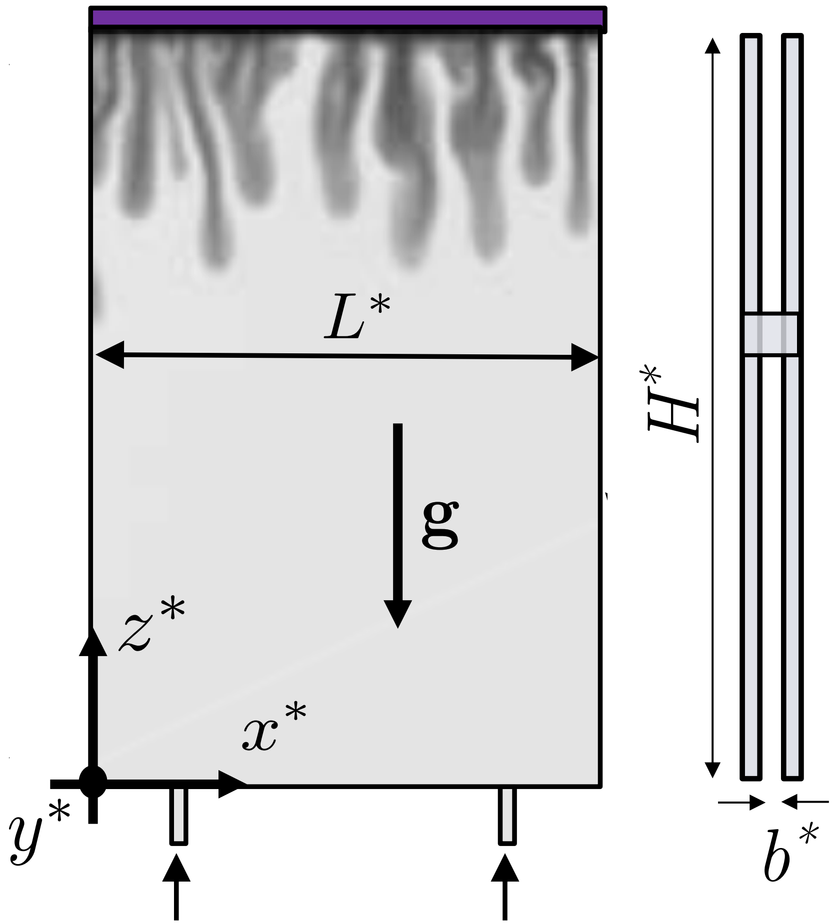

$$w(y) = W_z \left[\left(\frac{2y}{b} \right)^2 - 1 \right]$$

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

Laminar Poiseuille channel flow

Cell equivalent permeability $k = \dfrac{b^2}{12}$

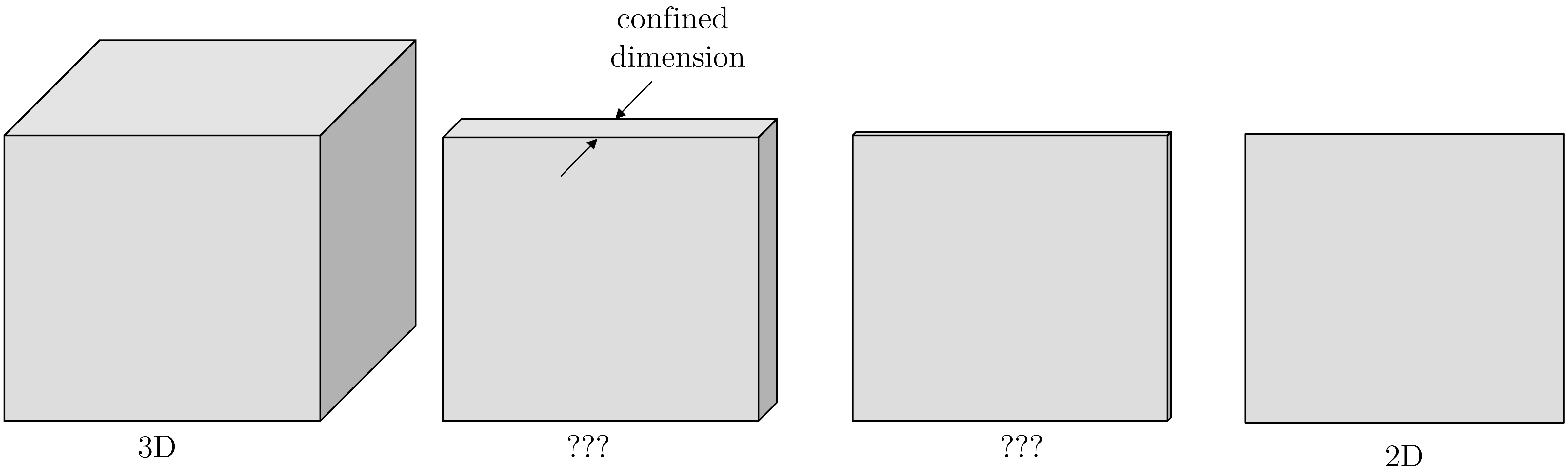
$$\frac{\mu}{k} w = -\frac{\partial p}{\partial z}$$

$$w = \frac{k}{\mu} \left| \frac{dp}{dz} \right|$$

Darcy law

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

Dimensional transition: Hele-Shaw flow



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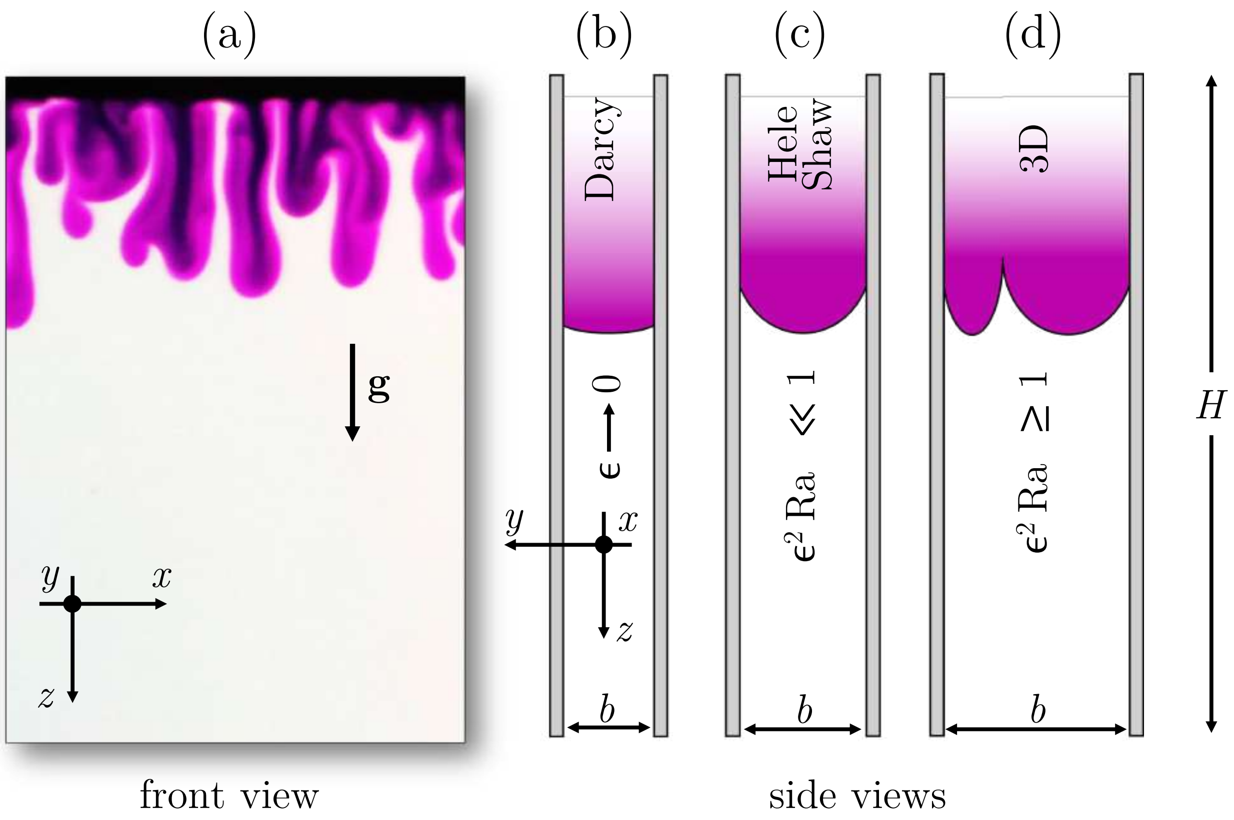
Perturbative corrections for the scaling of heat transport in a Hele-Shaw geometry ...

Juvenal A. Letelier[1,2,†], Nicolás Mujica[3] and Jaime H. Ortega[4]



$$0 = -\nabla p - \boldsymbol{u} + T\hat{z} + \frac{6}{5}\epsilon^2\nabla^2\boldsymbol{u} - \frac{2}{35}\epsilon^2 Ra(\boldsymbol{u}\cdot\nabla T)\hat{z}$$

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

2D Simulations

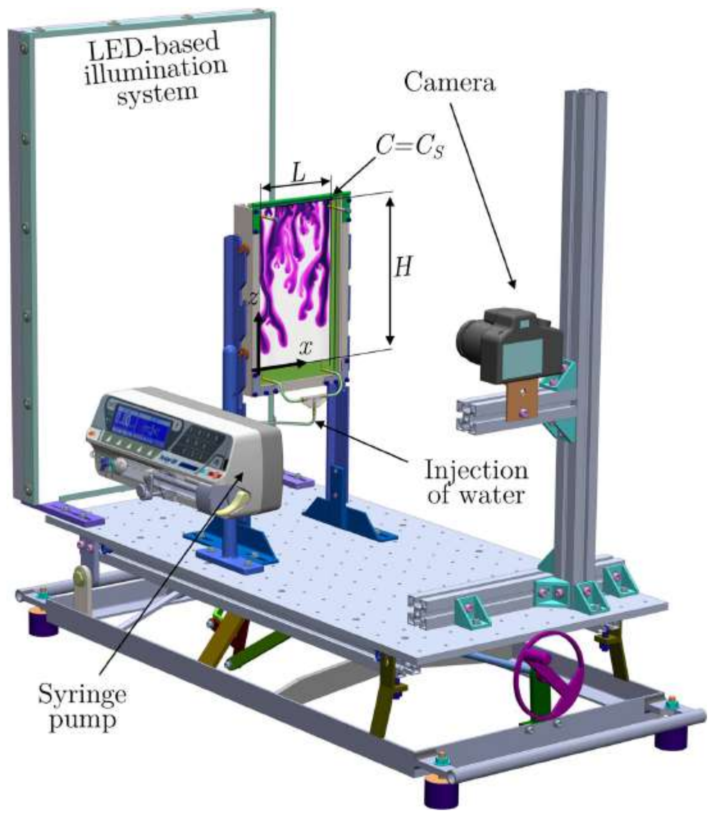
Experiments

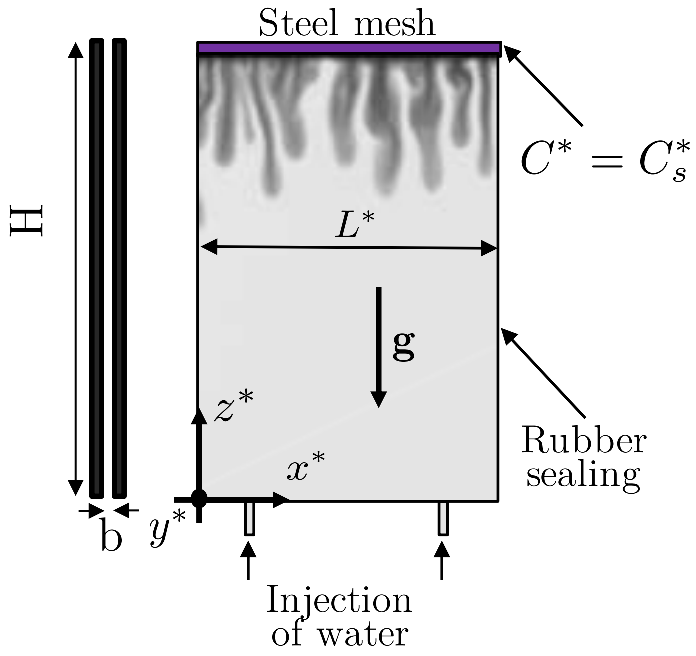
anisotropy ratio $\epsilon = b^*/\sqrt{12}H^*$

Rayleigh number $Ra = \dfrac{g\Delta\rho_s^*(b^*)^2H^*}{12\mu D}$

Possible explanation reconciling Hele-Shaw experiments and simulations

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





fluid

$\Delta\rho_S^*$=45 kg/m^3
D=1.7×10^{-9}m^2/s
μ=9.2×10^{-4} Pa s

geometry

b^*∈[0.1;1] mm
H*∈[105;343] mm
L* = 200 mm

- Acquisition rate: 1 fps, 24 Mpx
- KMnO4 in water
- Linear dependency $\rho^*(C^*)$

$$\epsilon = b^*/\sqrt{12}H^*$$

$$Ra = \frac{g\Delta\rho_s^*(b^*)^2H^*}{12\mu D}$$

Ra varied with b^* and H^*

Ra ∈ [4.6×10^4 ; 6.7×10^6]

Slim et al., *Phys. Fluids* (2013)
Ching et al., *Phys. Rev. Fluids* (2017)

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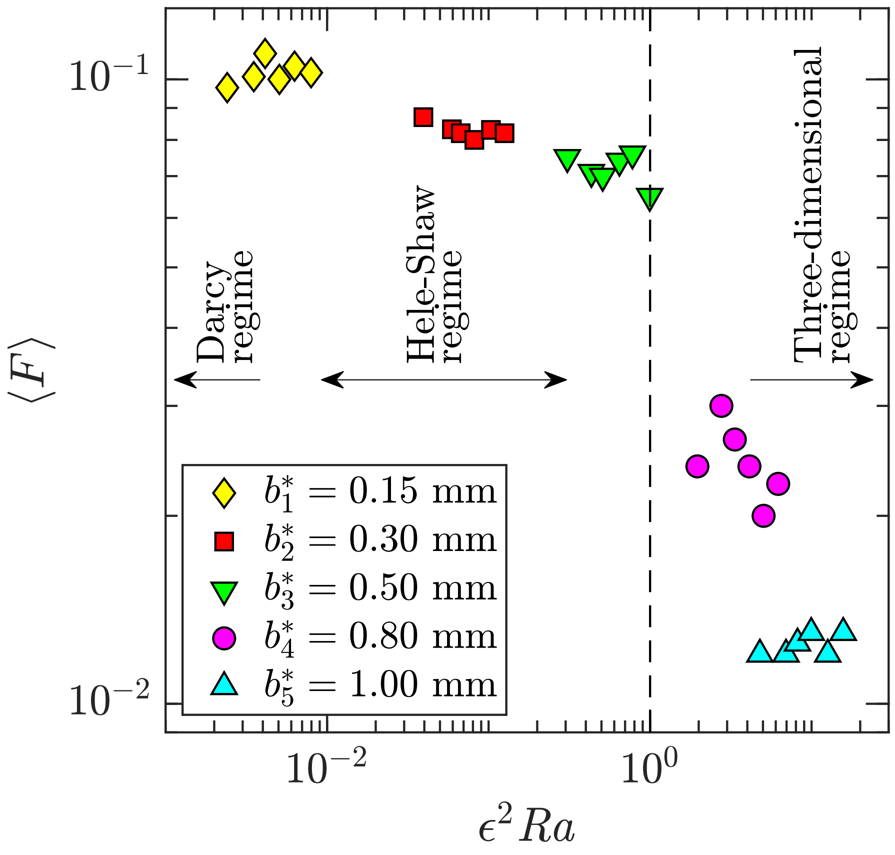

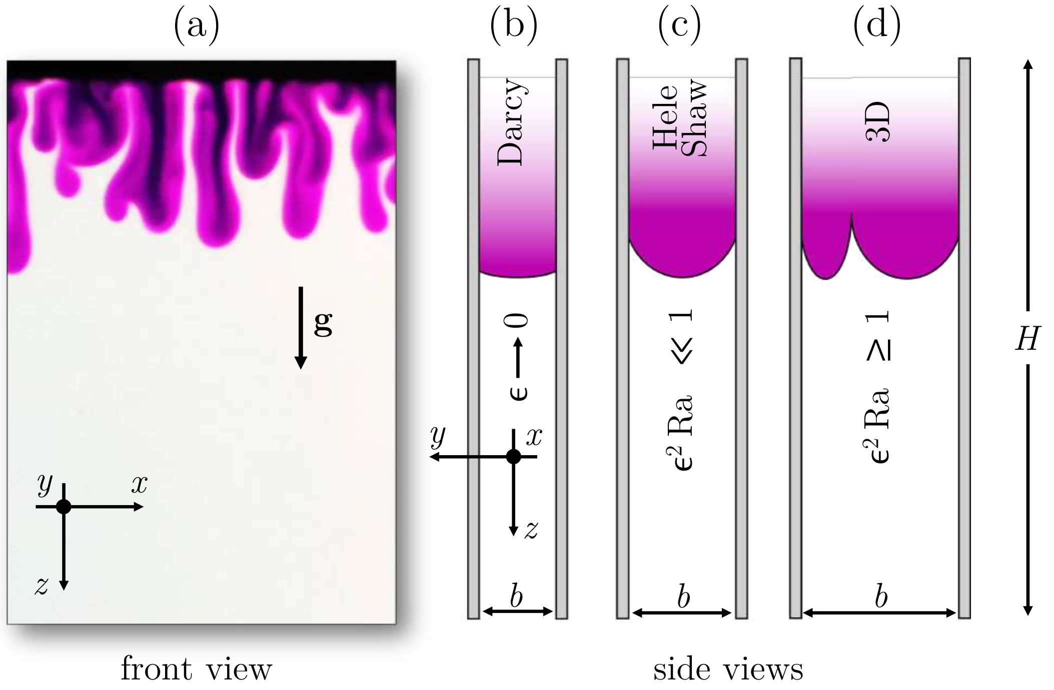

$$\epsilon^2 Ra \begin{cases} \to 0 \Rightarrow \text{Darcy flow} \\ \ll 1 \Rightarrow \text{Hele—Shaw flow} \\ > 1 \Rightarrow \text{three—dimensional} \end{cases}$$

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

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

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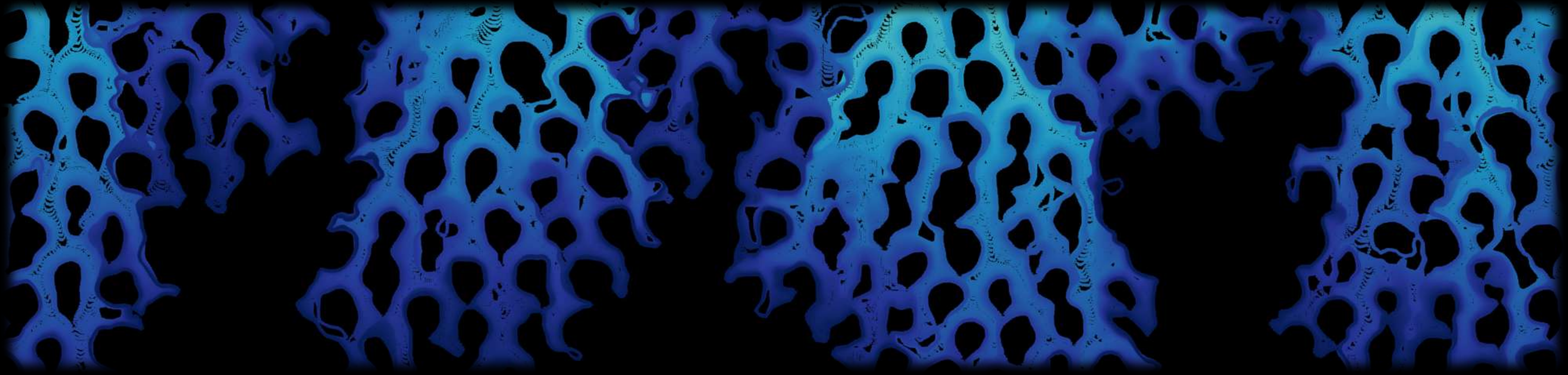

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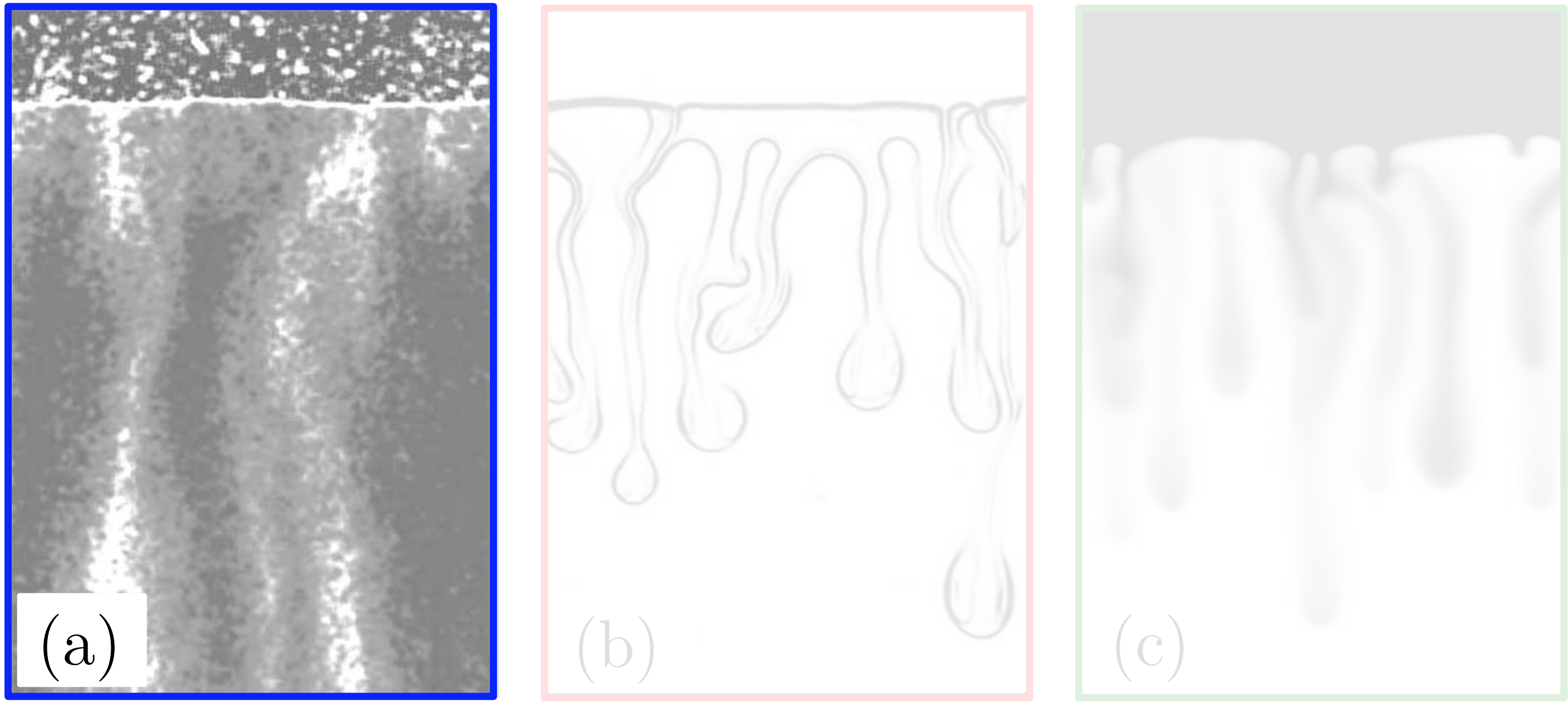

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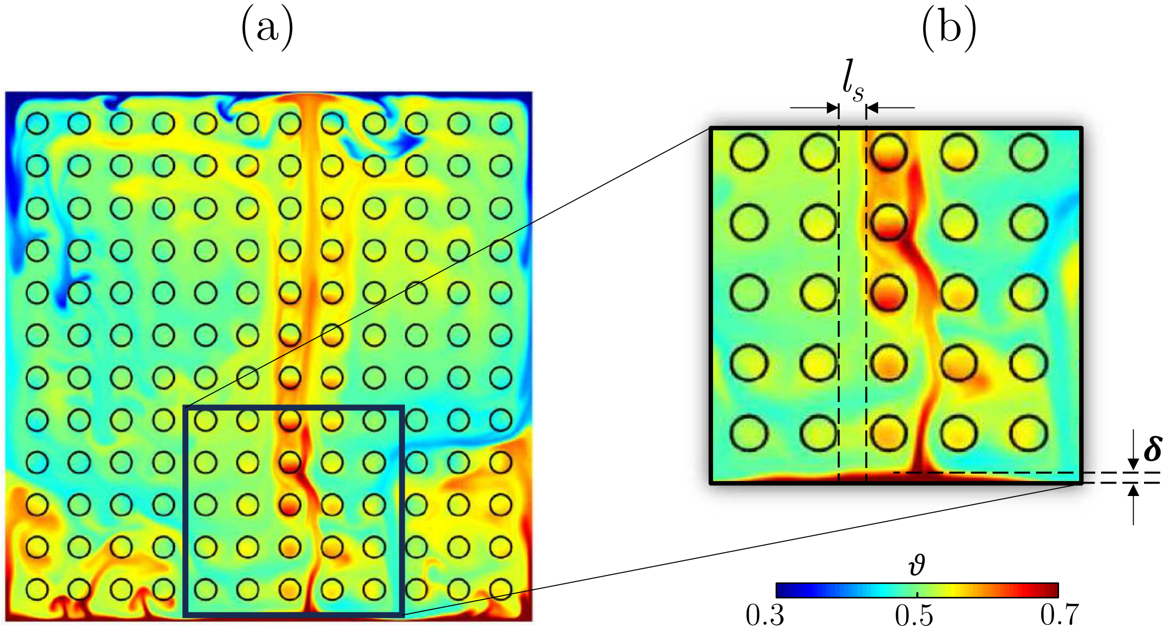
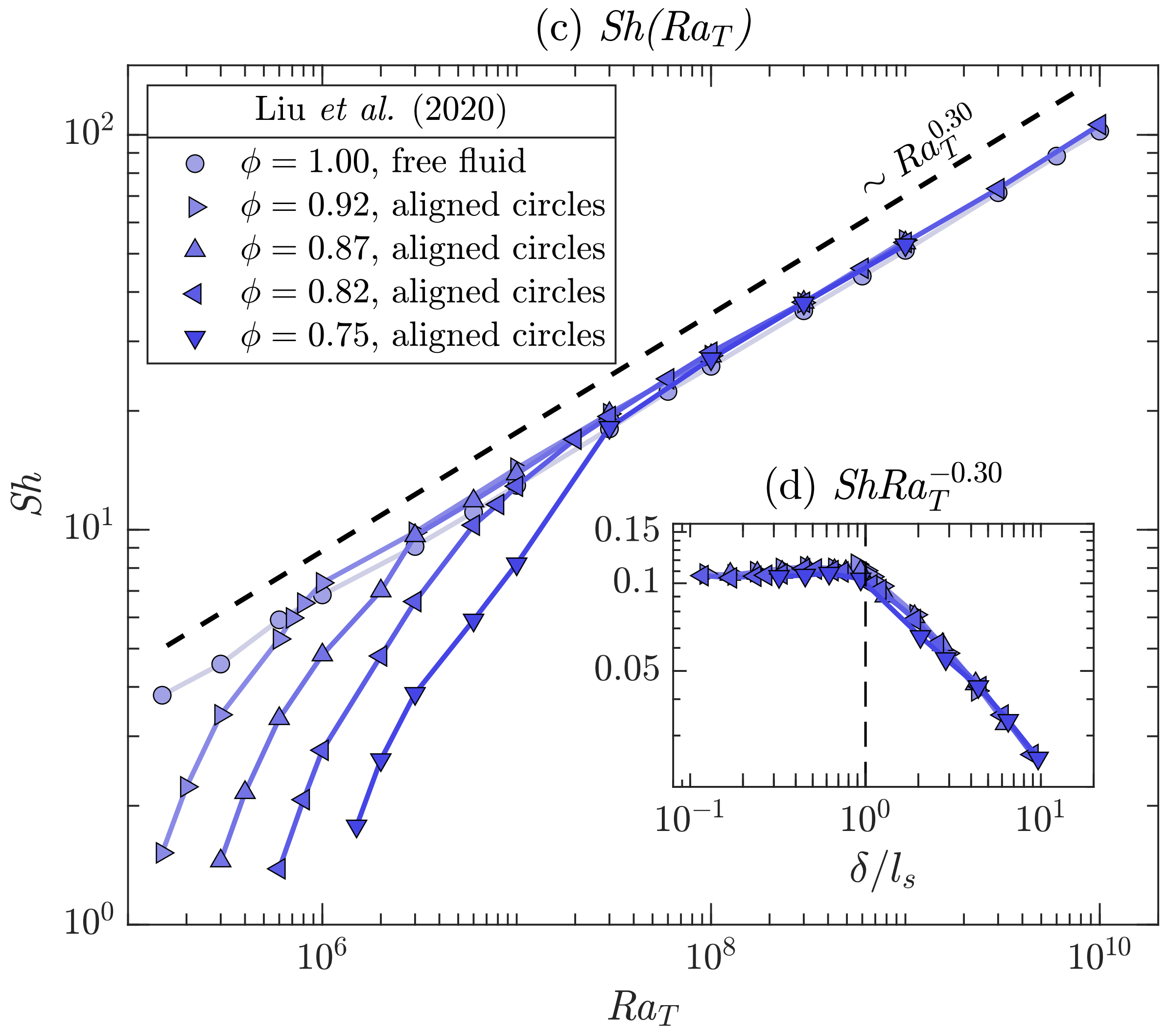
Pore-scale simulations

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





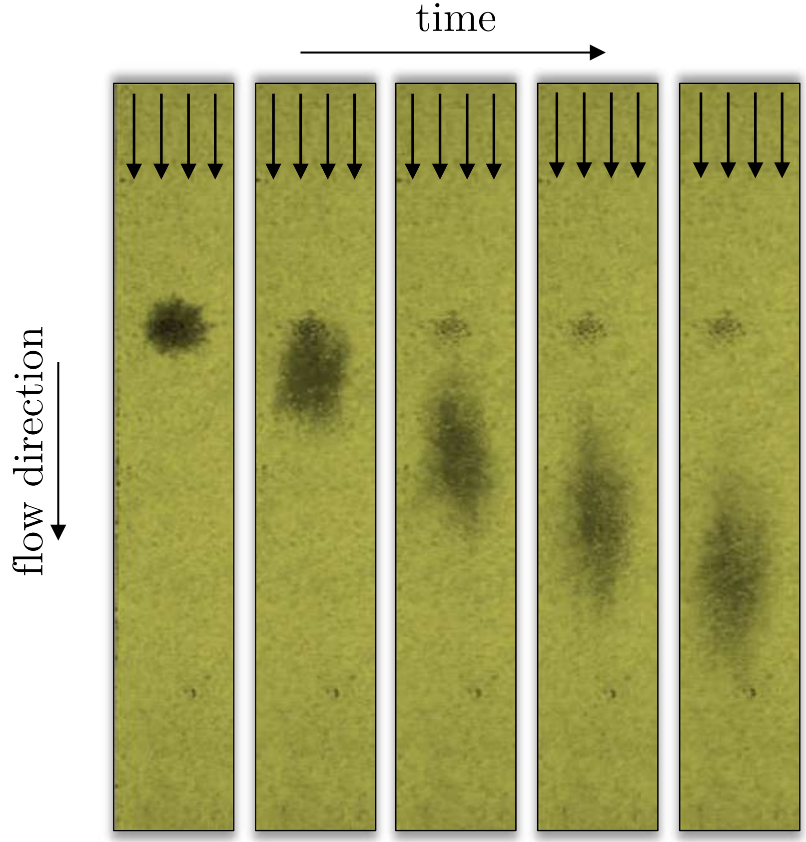
De Paoli https://arxiv.org/abs/2310.01999

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

Influence of dispersion

Mechanism of dispersion

Patch of dye in a uniform flow through a porous medium



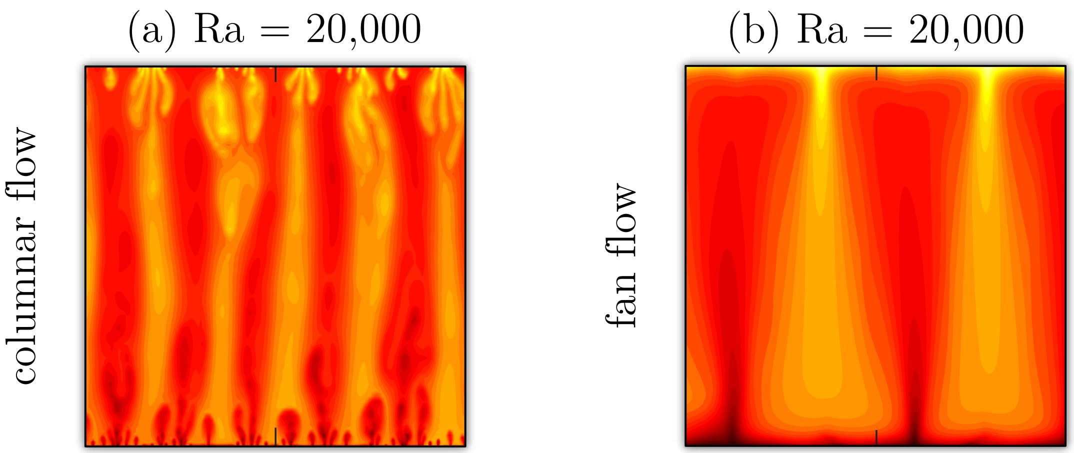
Woods, *Flows in porous rocks* (2015)

Darcy formulation of dispersion

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

Fickian formulation for dispersion

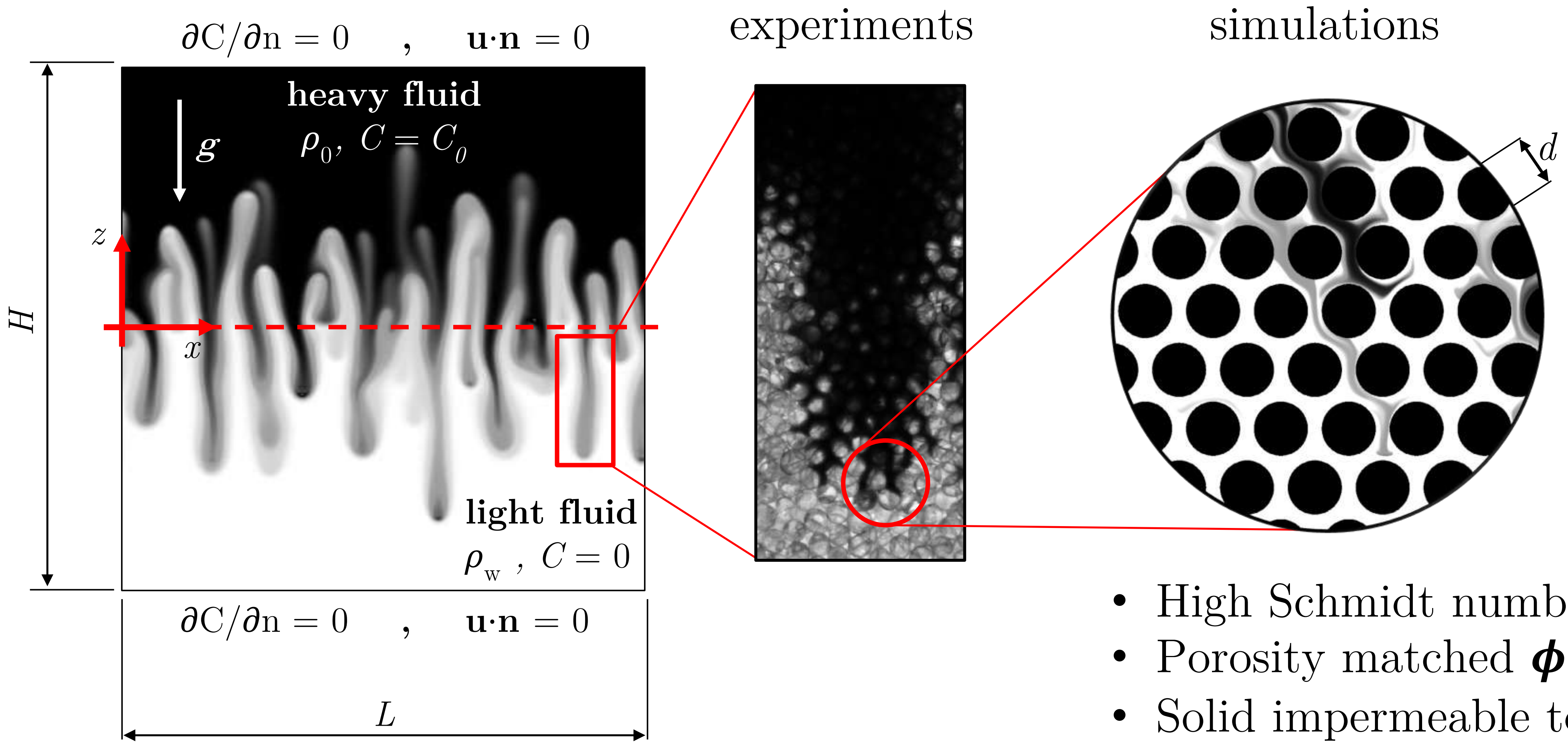
$$\mathbf{D} = D\mathbf{I} + (\alpha_L - \alpha_T)\frac{\mathbf{uu}}{|\mathbf{u}|} + \alpha_T \mathbf{uI},$$



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

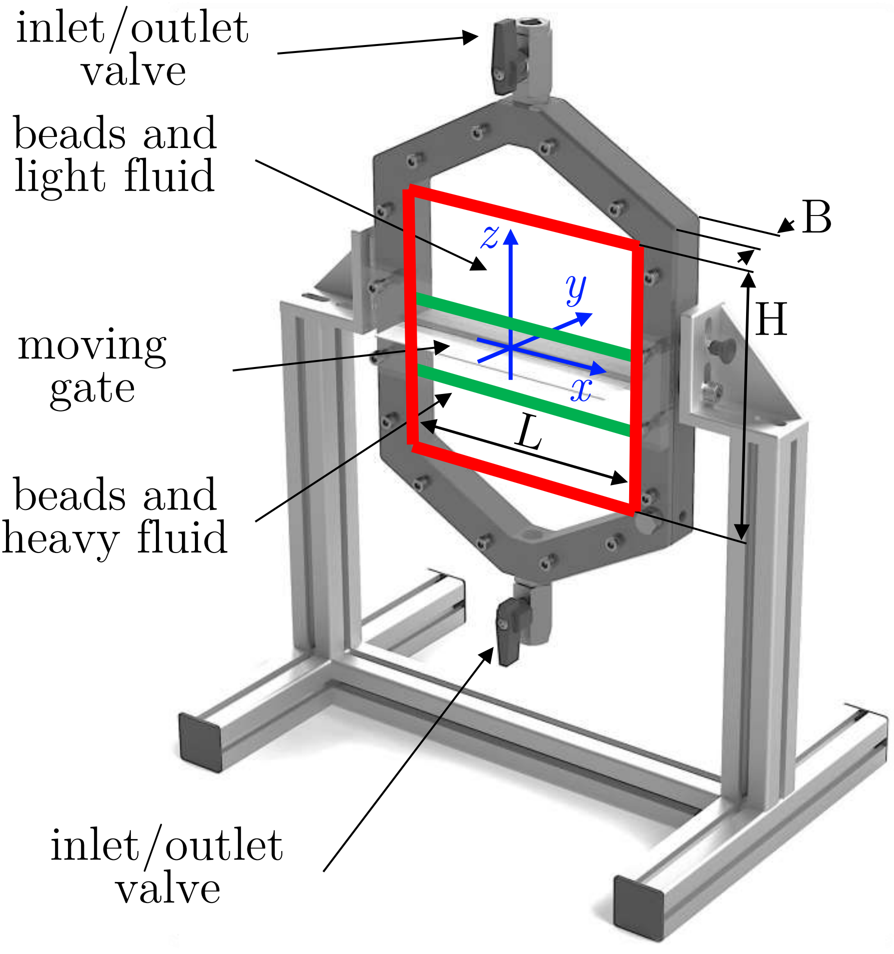
These models required validation: Experiments and simulations in porous media

Flow configuration

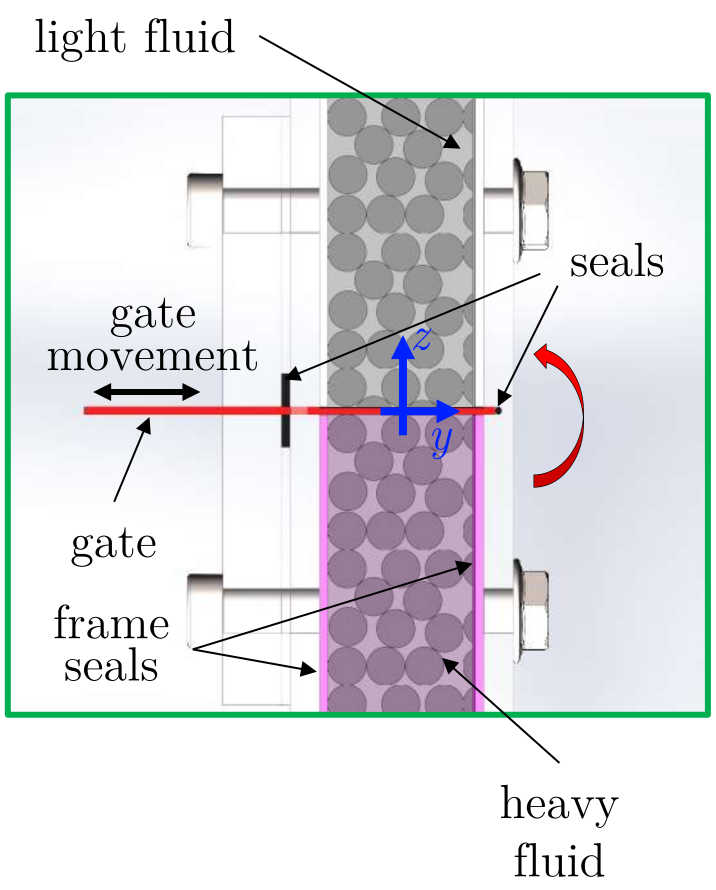


- High Schmidt number
- Porosity matched $\phi = 0.37$
- Solid impermeable to solute
- Linear dependency $\rho(C)$

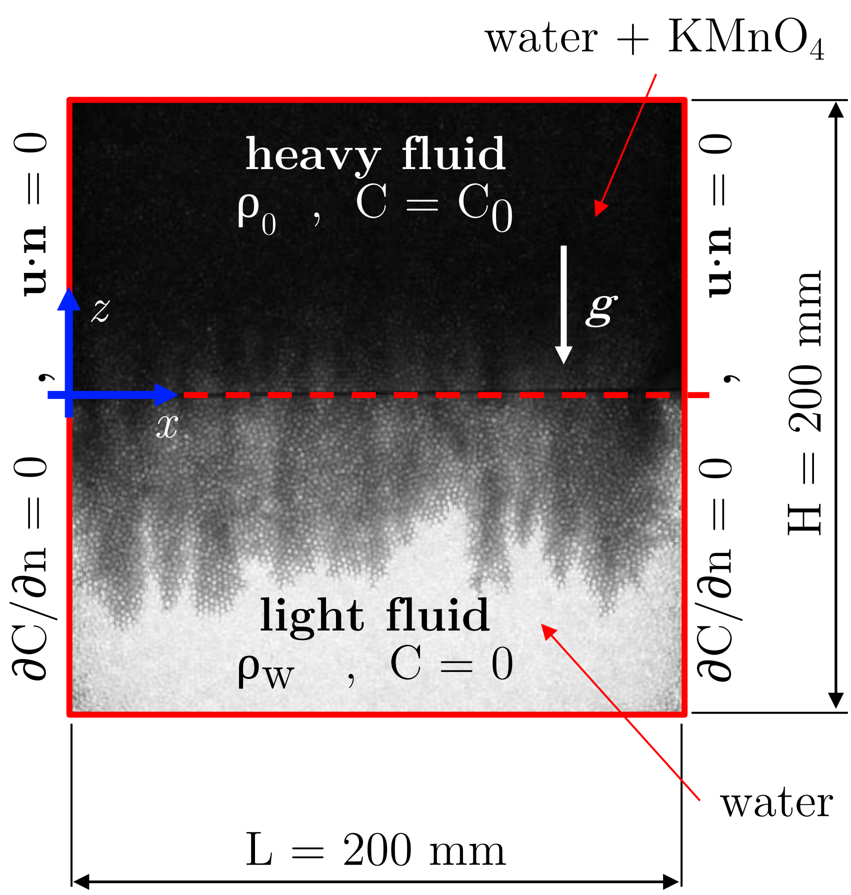
(a) Hele-Shaw cell

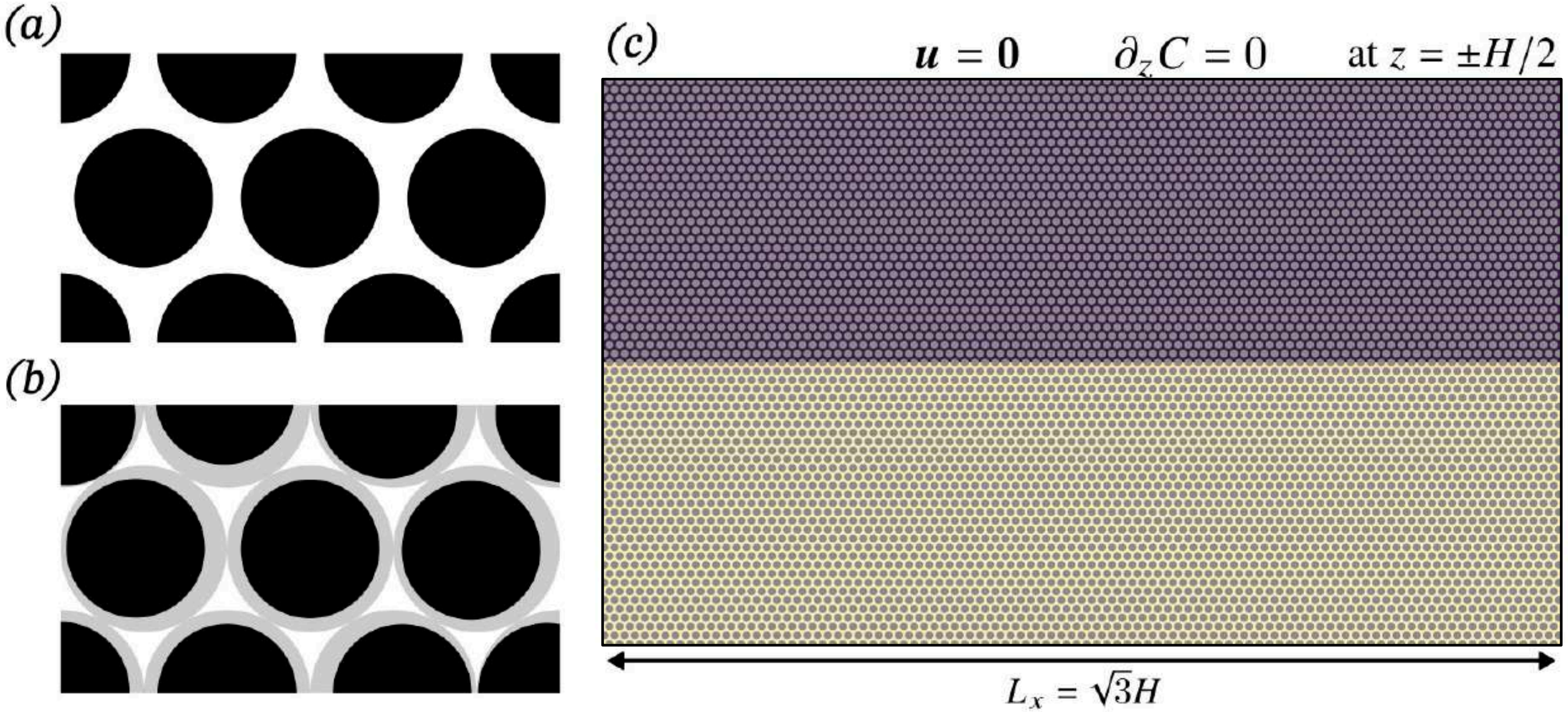


(b) gate (side view)



(c) measurement region





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

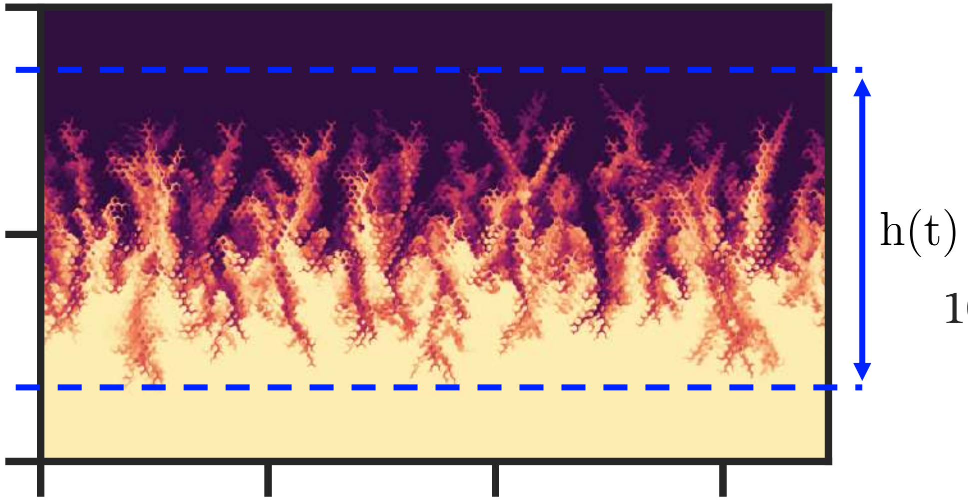
$$\partial_t C + (\boldsymbol{u} \cdot \boldsymbol{\nabla}) C = D \nabla^2 C,$$

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

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

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

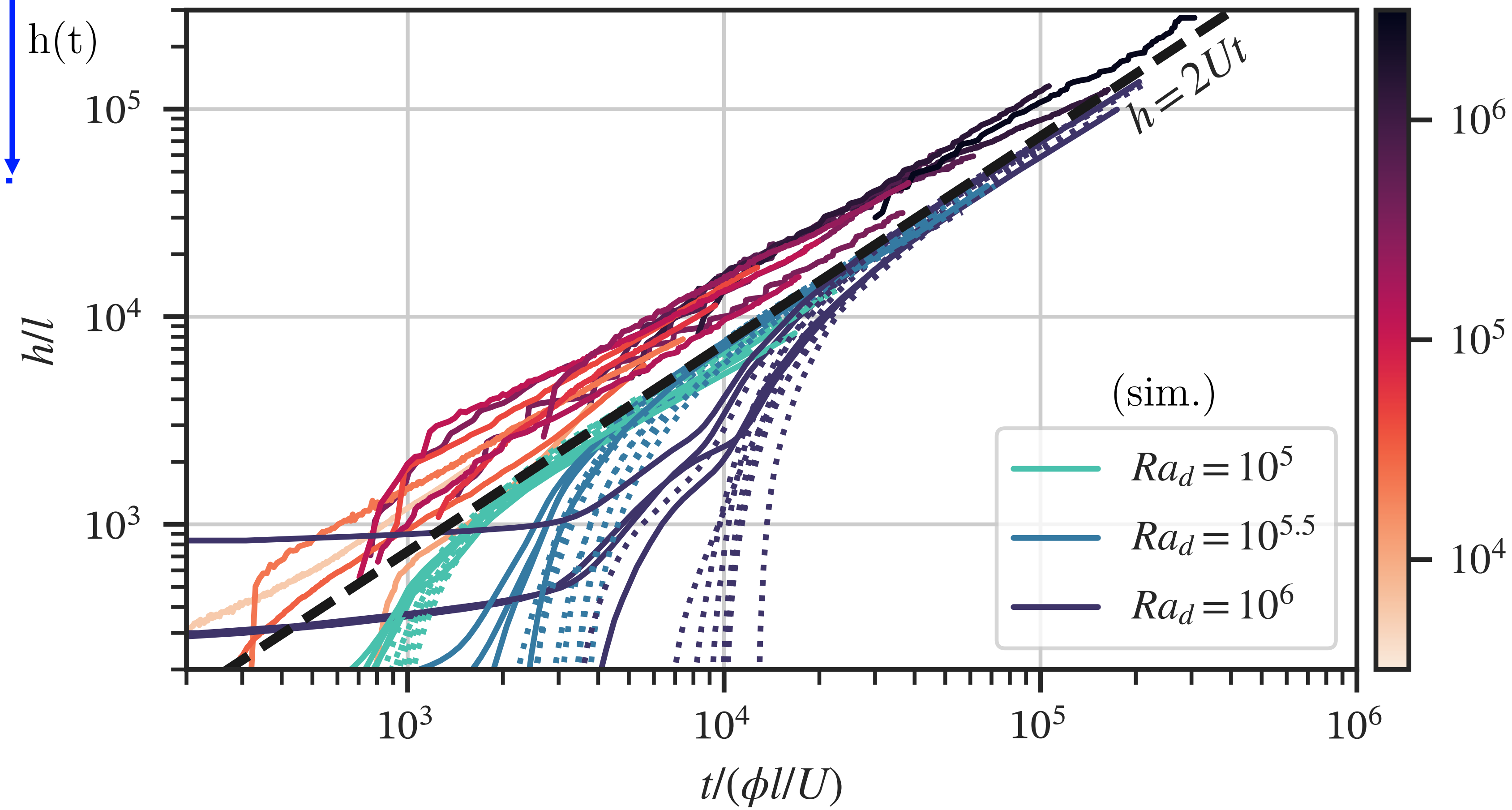
Mixing length



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

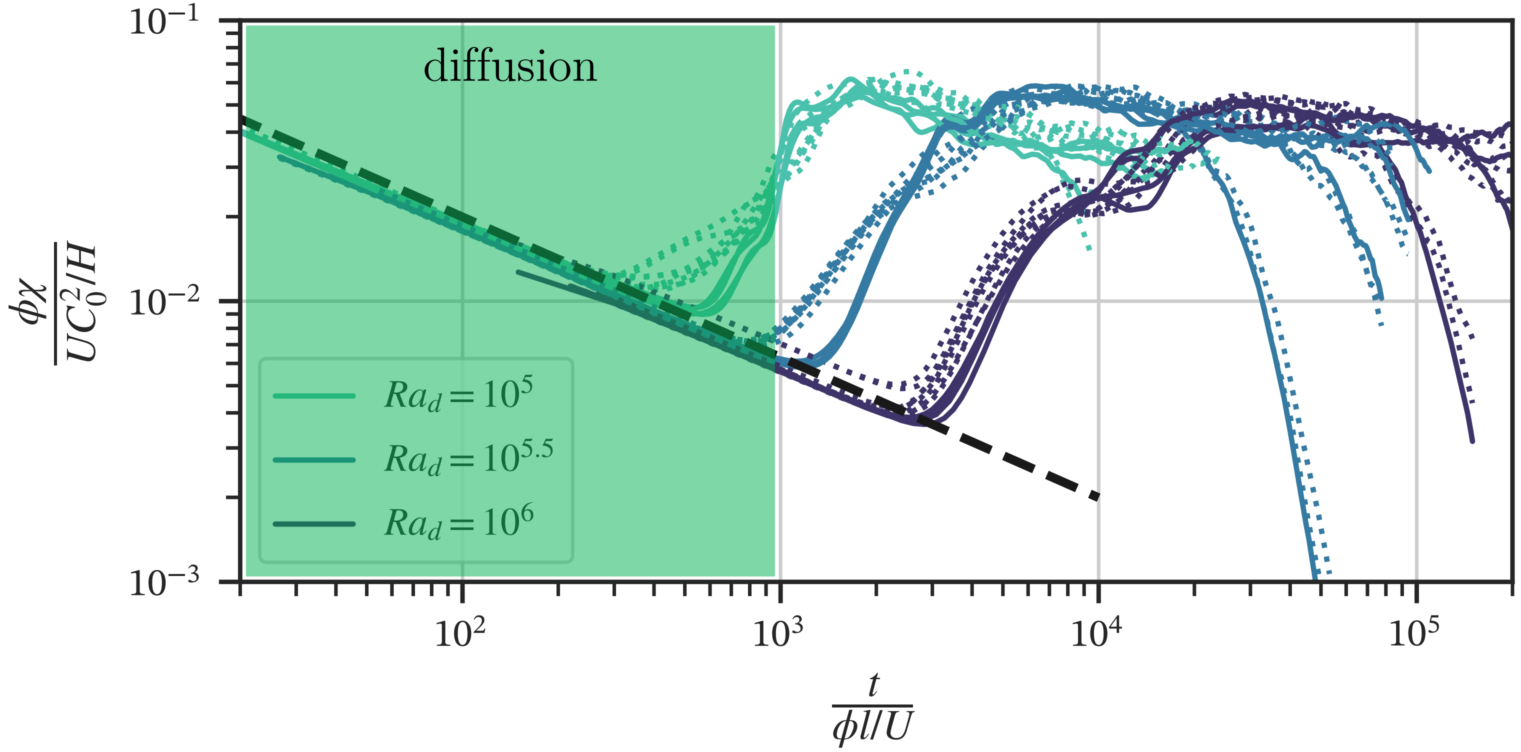
$$\ell = \frac{\phi D}{U}$$

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



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

Can we model this mixing/dissolution process?



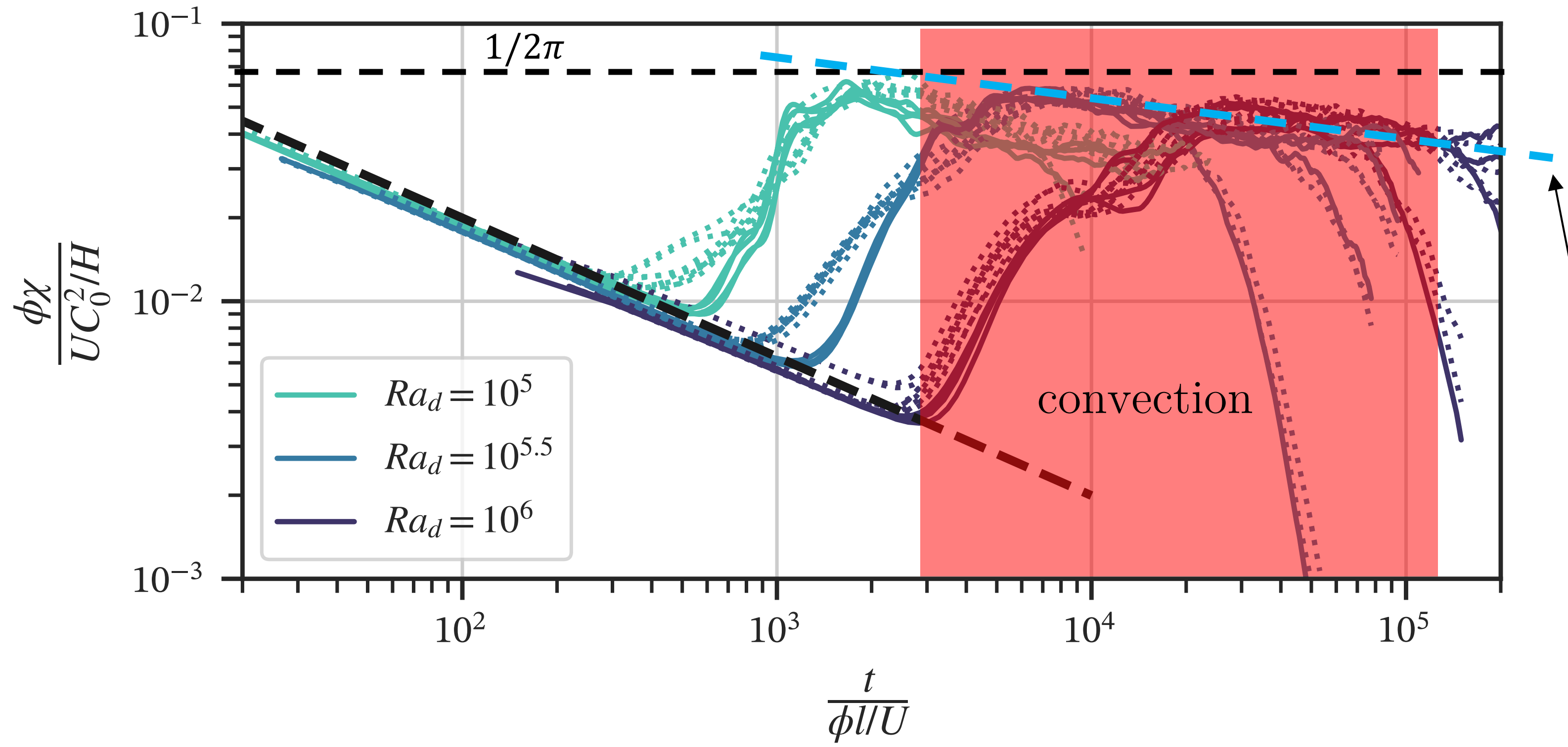
Diffusion:

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

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

$$\chi = \kappa\langle|\nabla C|^2\rangle = \frac{\kappa}{H}\int_{-\infty}^{\infty}|\partial_z C|^2 \mathrm{d}z = \sqrt{\frac{\kappa}{8\pi t}}\frac{(\Delta C)^2}{H}$$

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



Convection

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

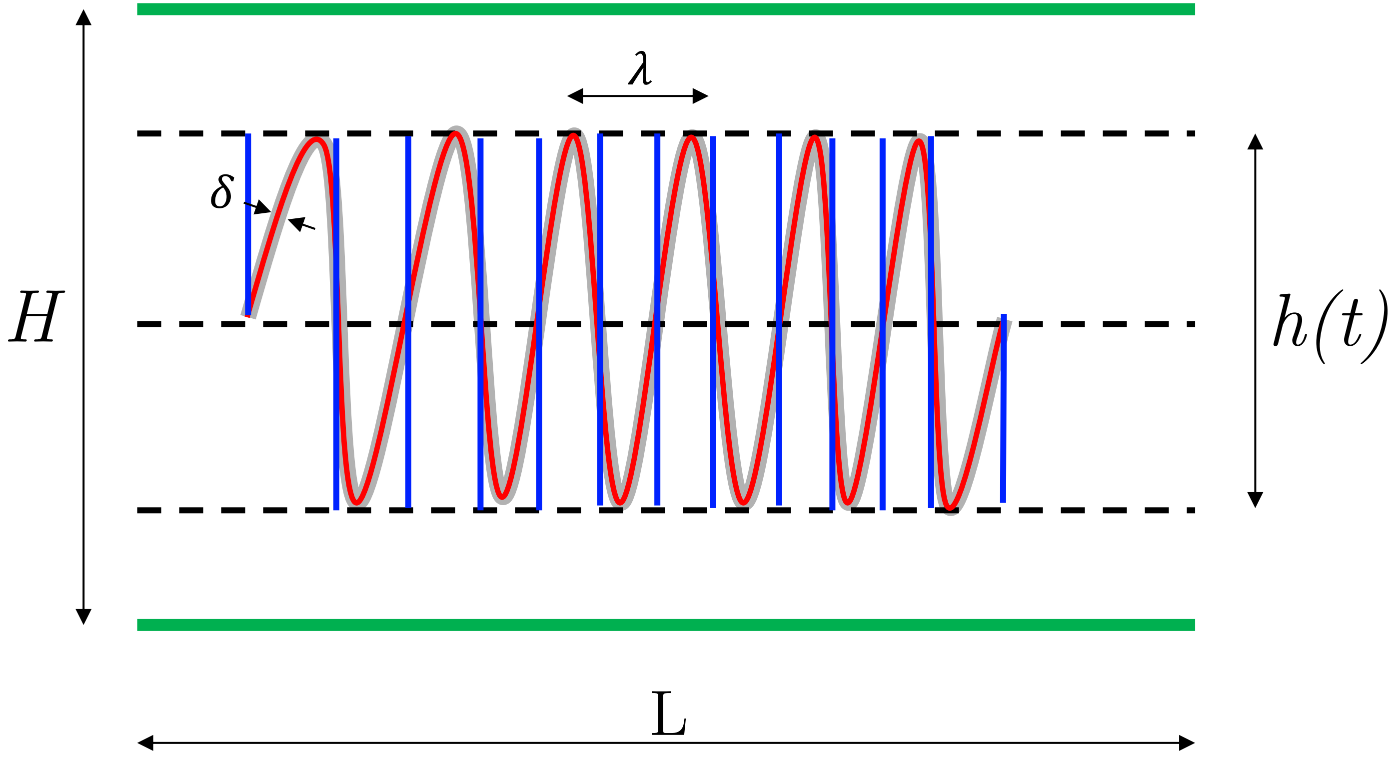
$$|\nabla C| \approx \frac{\Delta C}{2\sqrt{\pi\kappa t}}.$$

$$L_m \approx 2Ut,$$

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

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

Modelling scalar dissipation



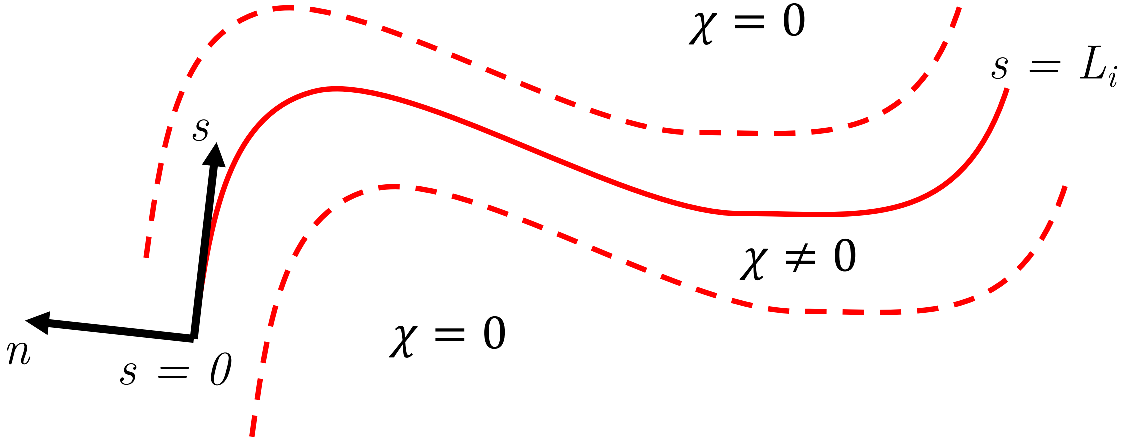
$$\chi = D\langle|\nabla C|^2\rangle = \frac{D L_i}{HL}\int_{-\delta/2}^{+\delta/2}|\partial_n C|^2\, dn$$

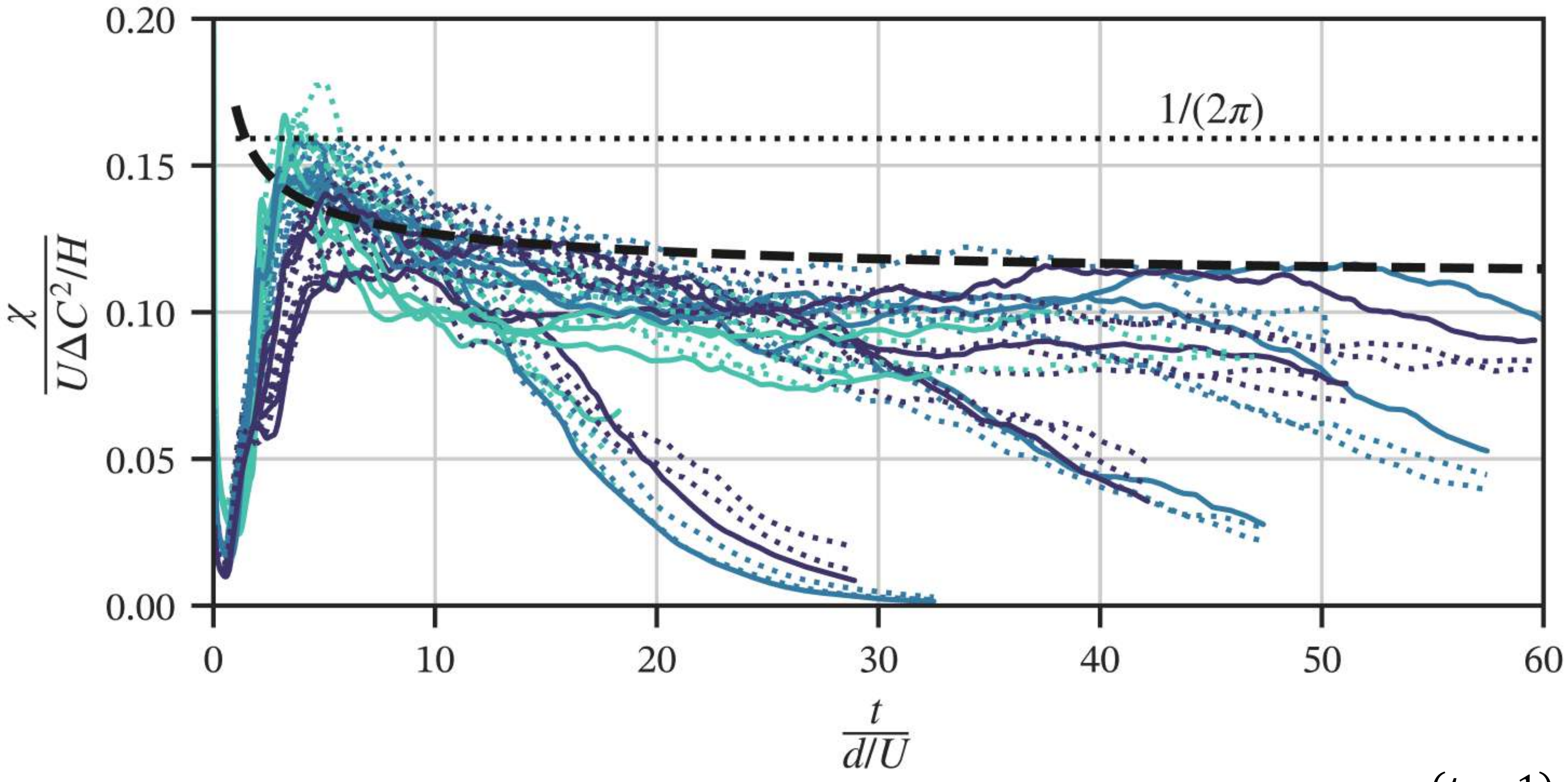
Assume:

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





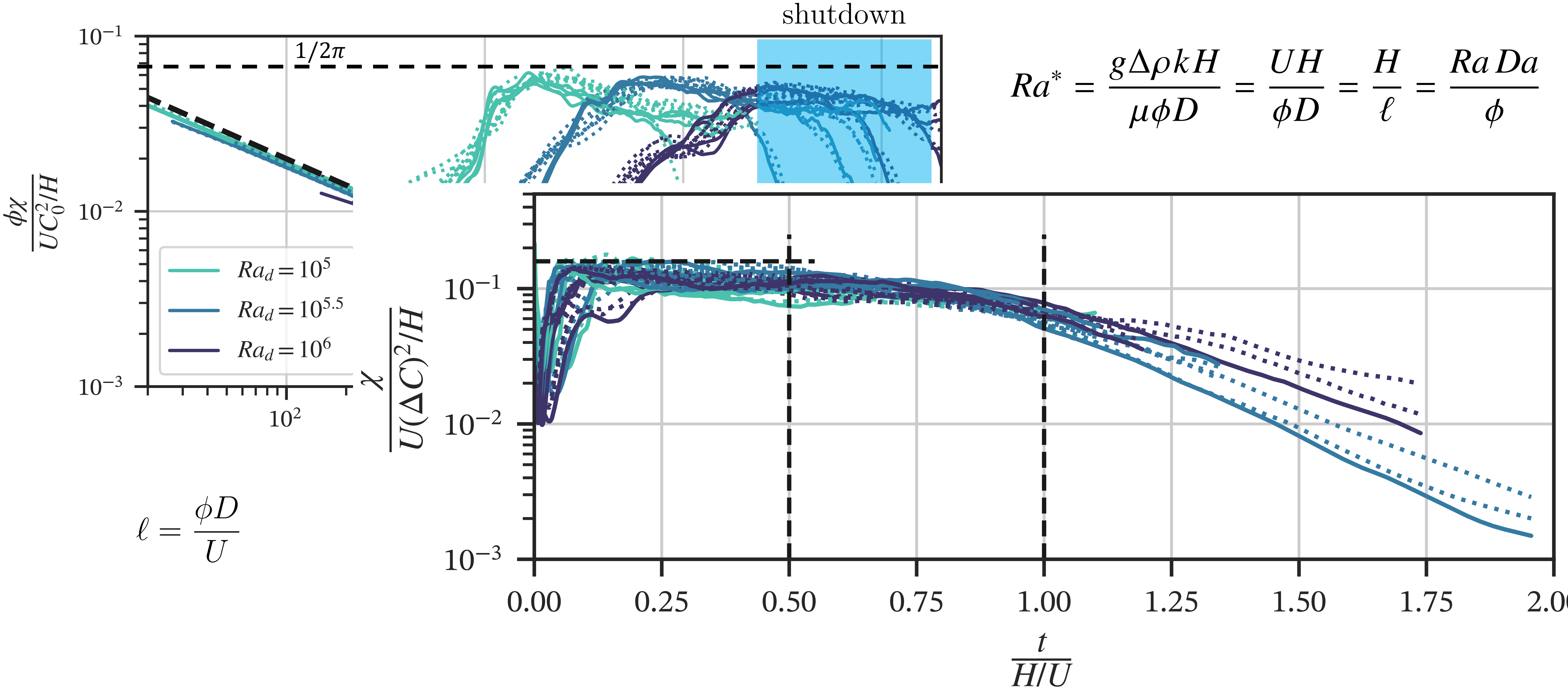
$1/2\pi$ is the maximum value of dissipation.

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

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



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

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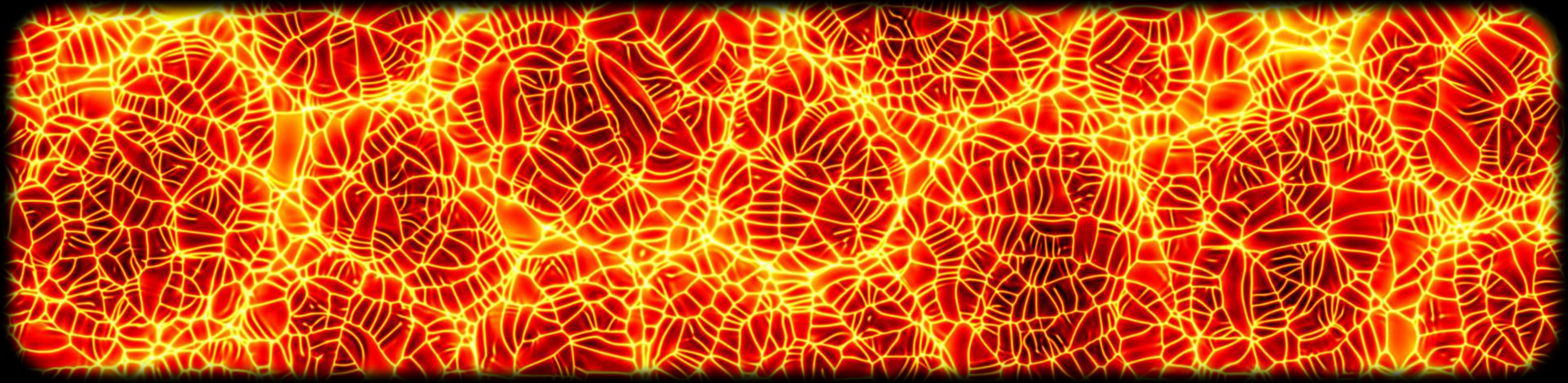
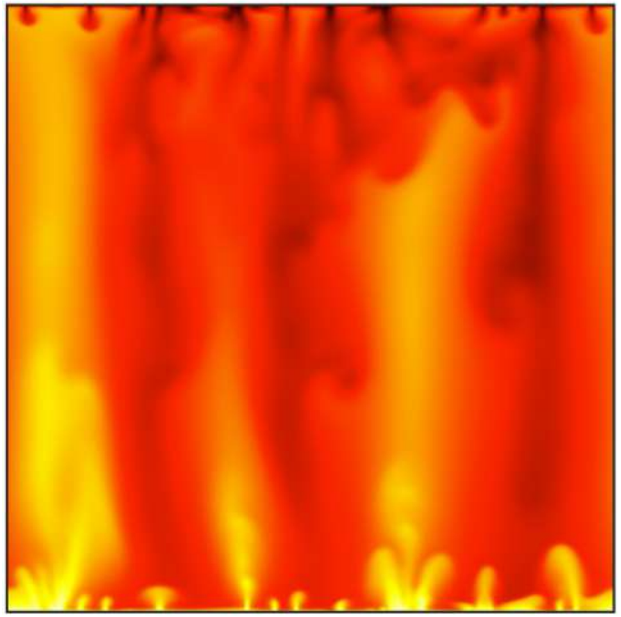
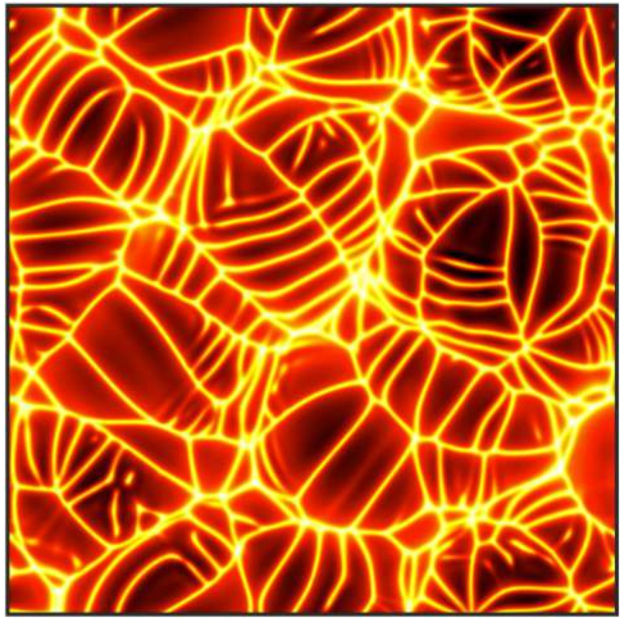


1. Convection in porous media is a **multiscale** and **multiphase** process
2. A **combination of experiments, simulations and theory** is required to model the flow dynamics
3. Recent developments in numerical and experimental capabilities enable measurements at unprecedented level of detail, but the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





pore-scale

https://arxiv.org/abs/2310.04068

review

https://arxiv.org/abs/2310.01999

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