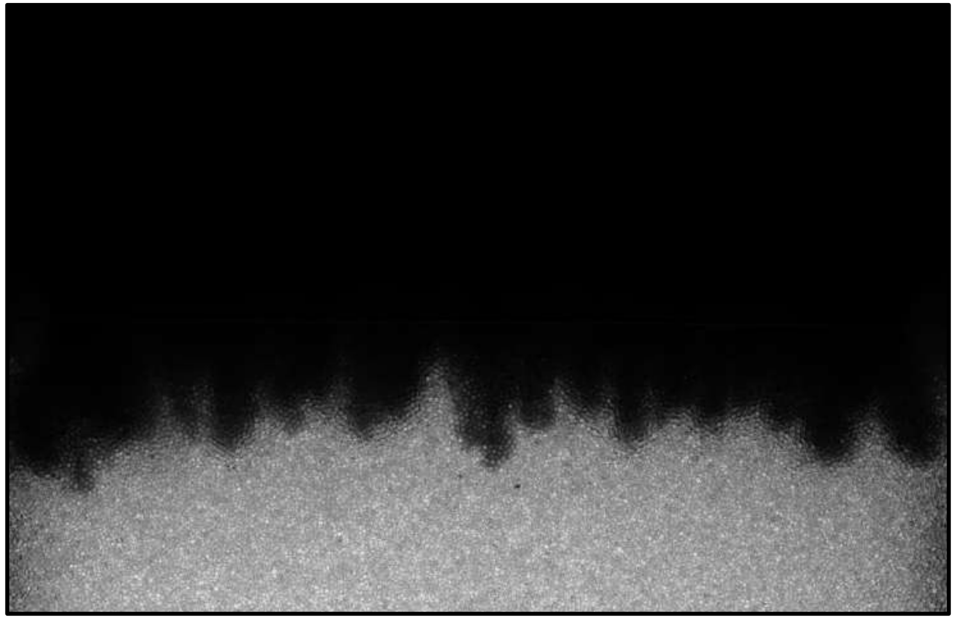
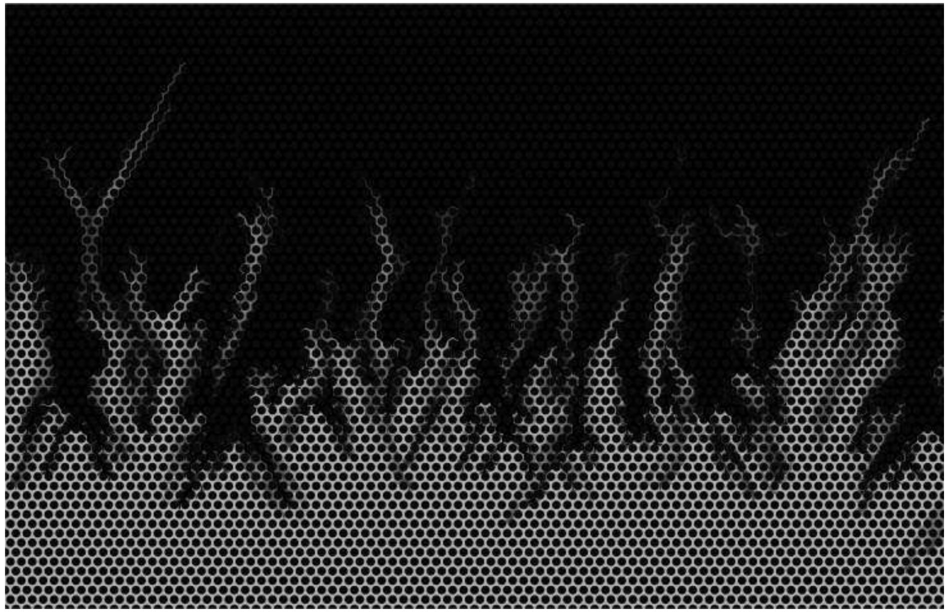
Pore-scale simulation of convective mixing in confined media





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gacm German Association for Computational Mechanics

September 10-13, 2023
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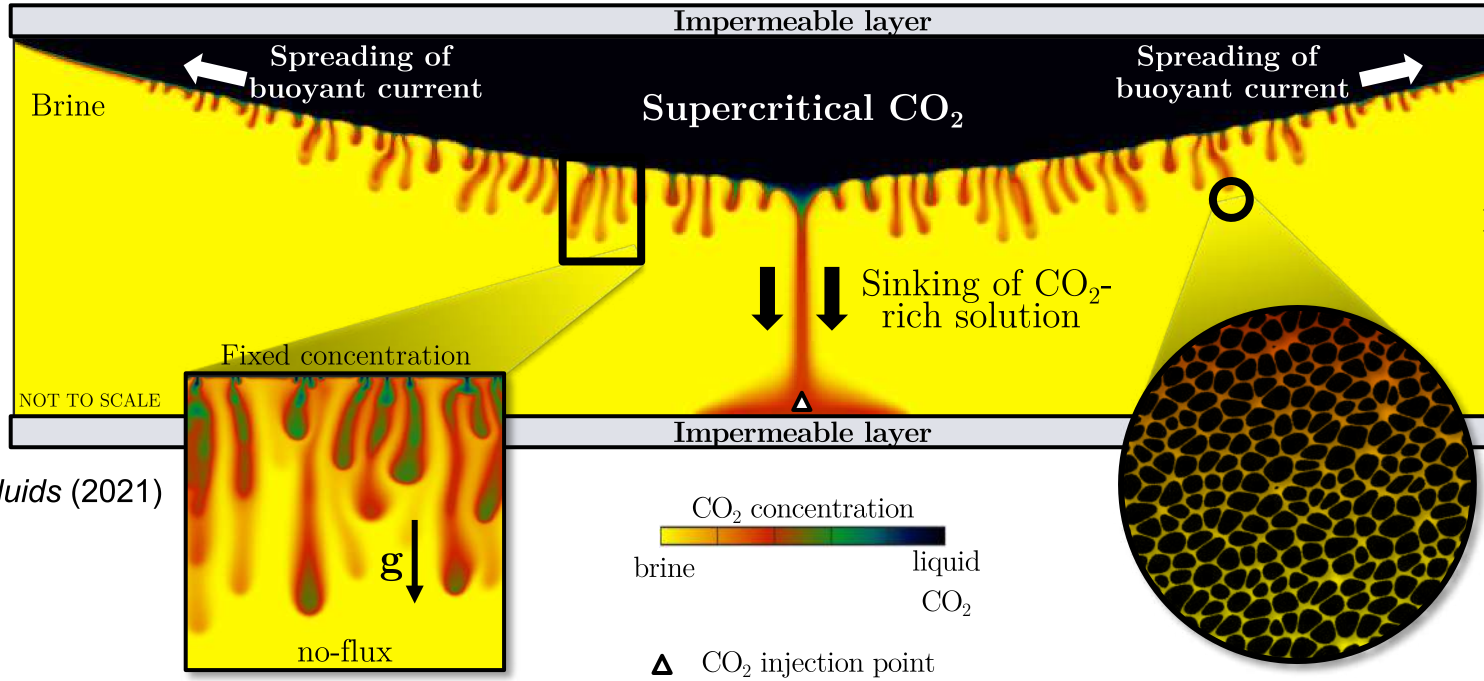
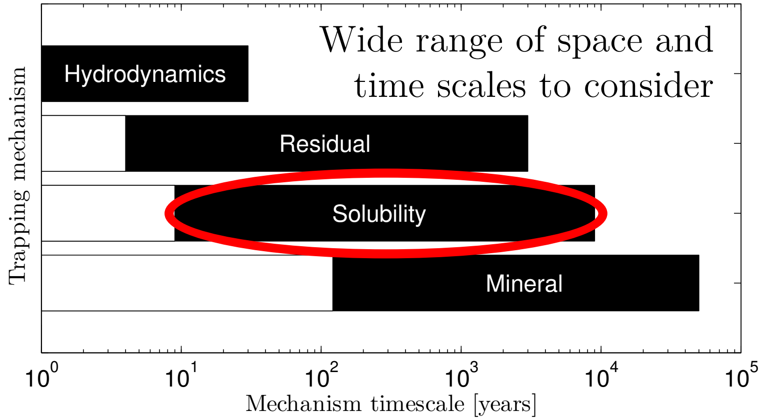
Carbon Capture and Storage

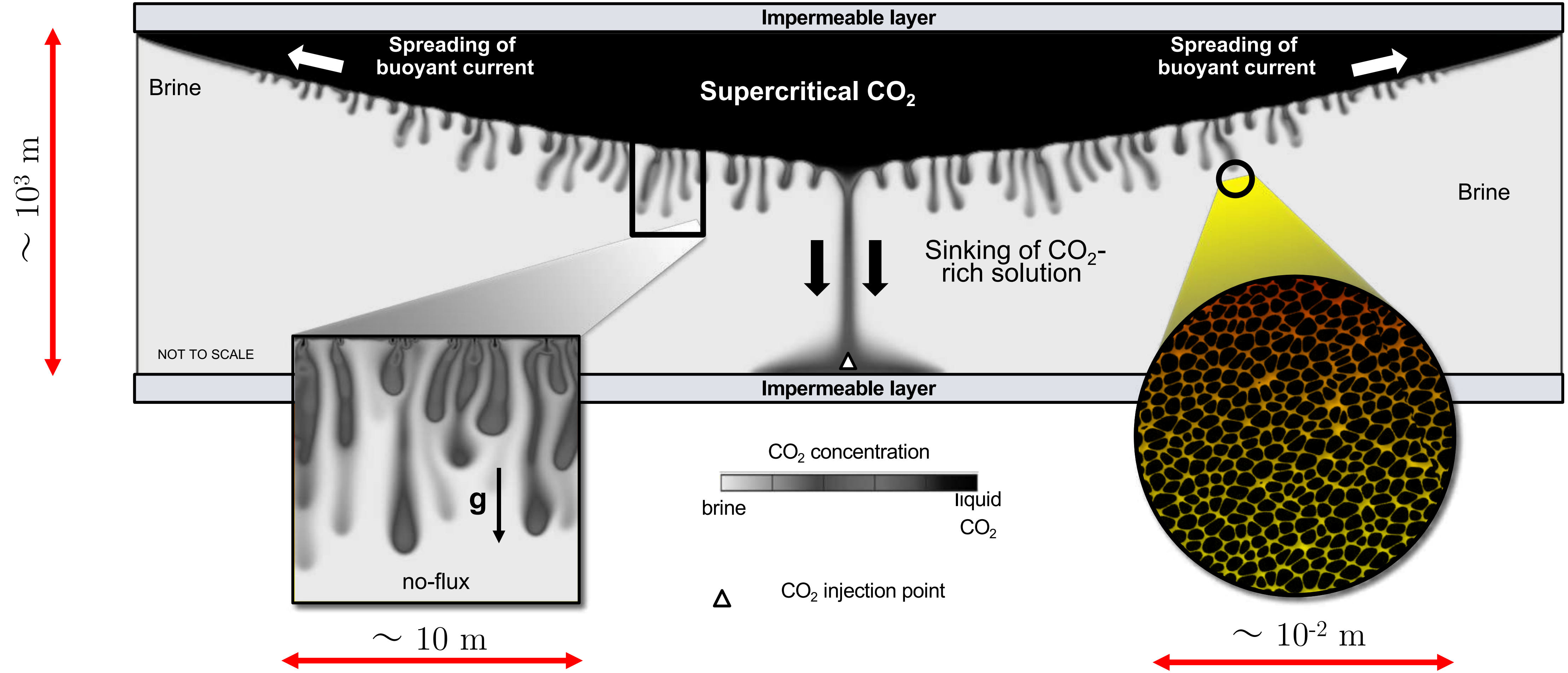


De Paoli, *Phys. Fluids* (2021)



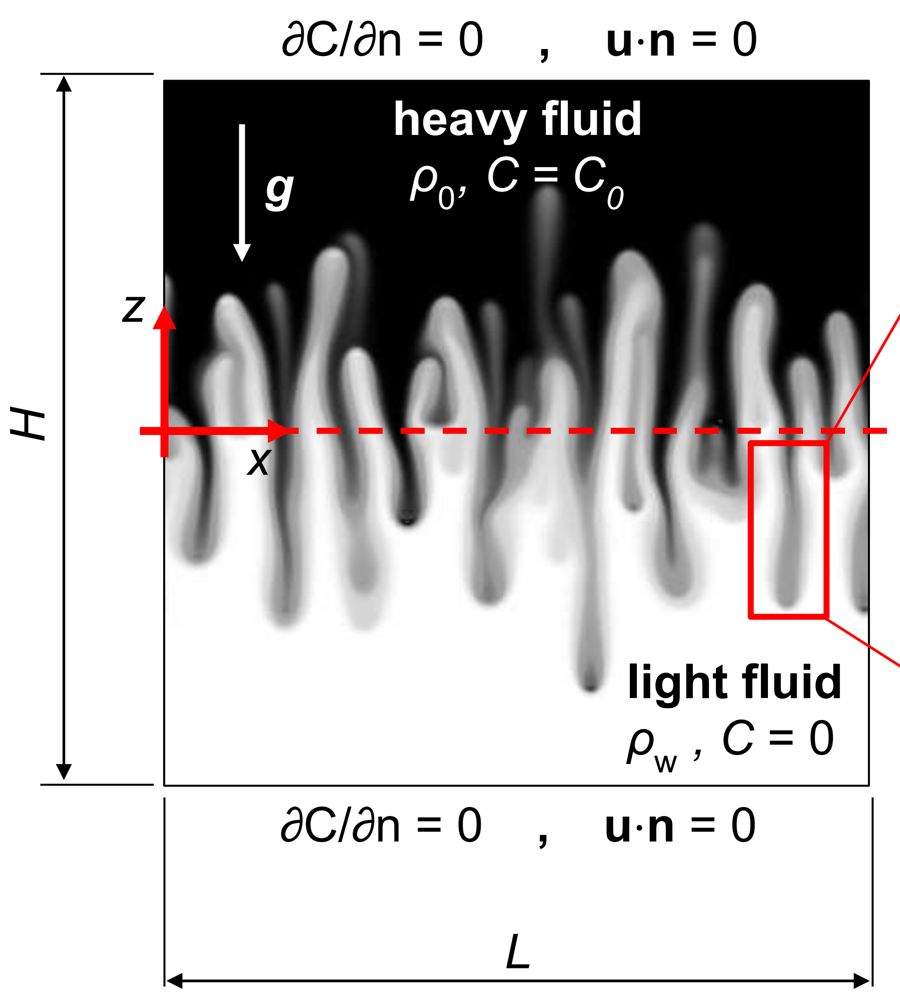
MacMinn et al., *Geophys. Res. Lett.* (2013)

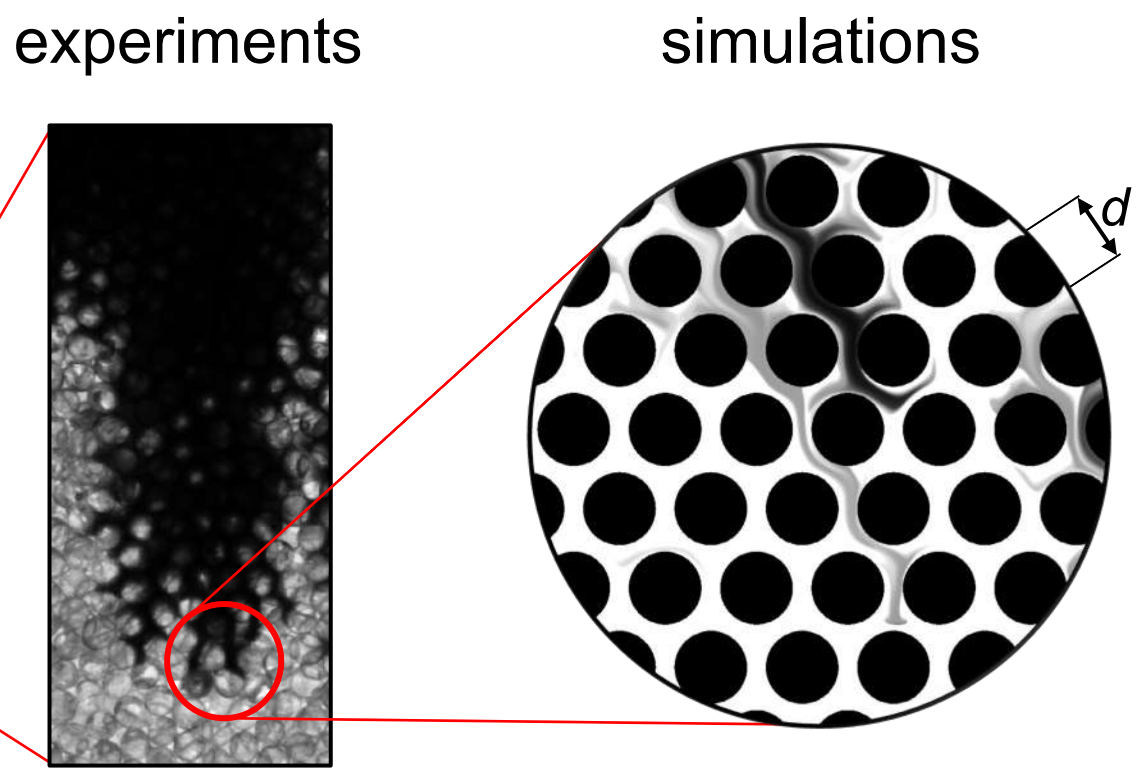
Convection in complex multiphase and multiscale systems



De Paoli, *Phys. Fluids* (2021)

Flow configuration

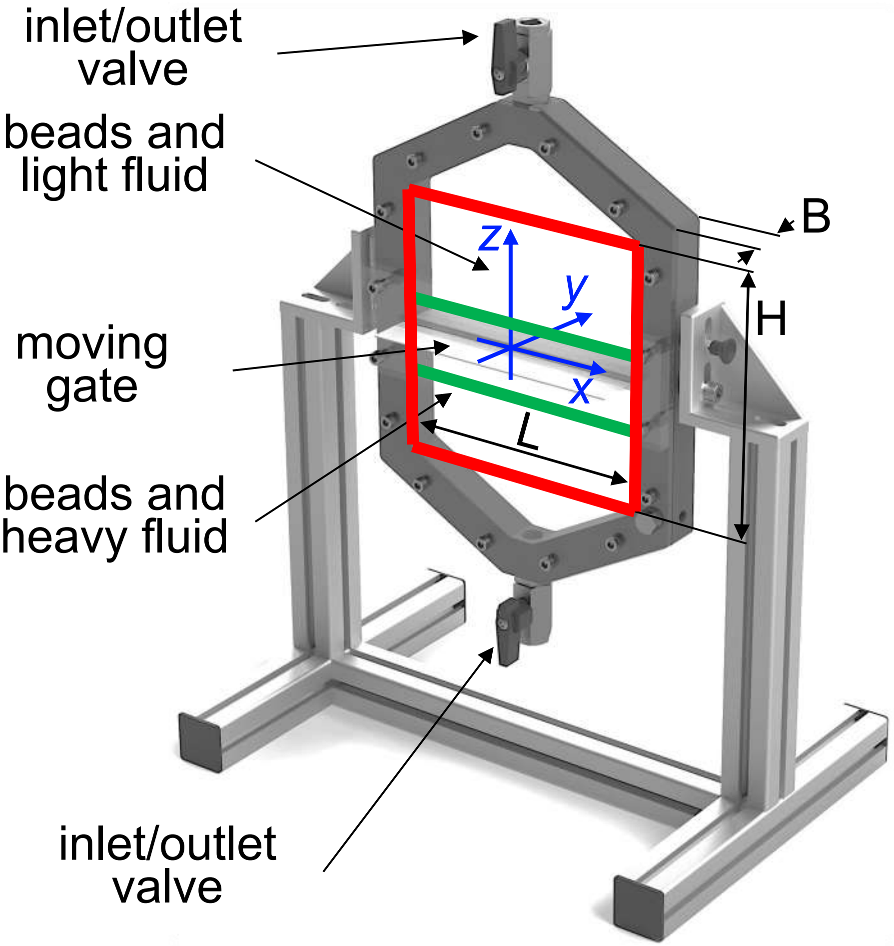




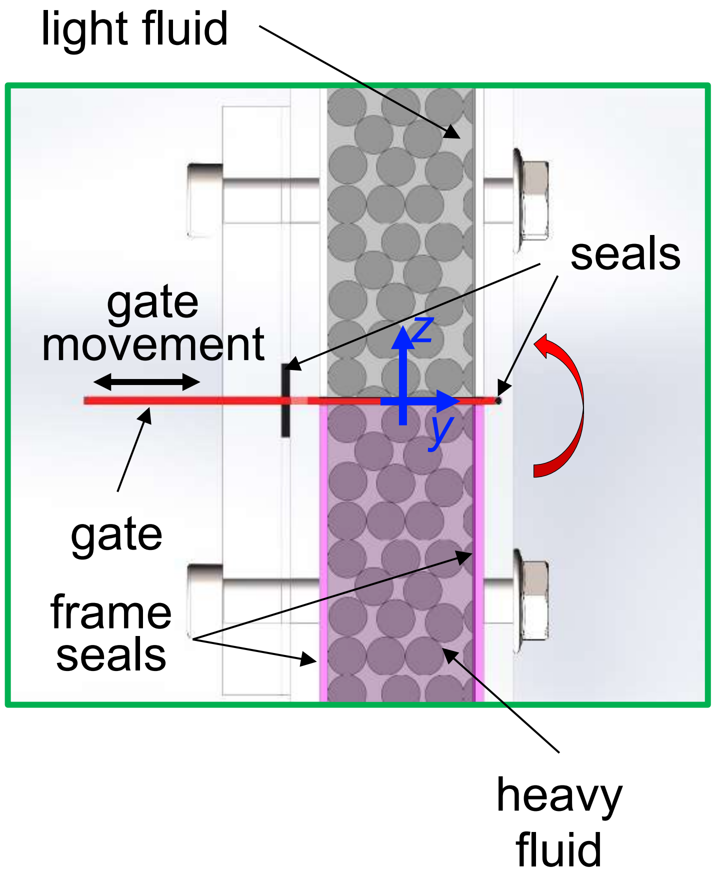
- High Schmidt number
- Porosity matched ϕ = 0.37
- Solid impermeable to solute
- Linear dependency $\rho(C)$

Experimental setup

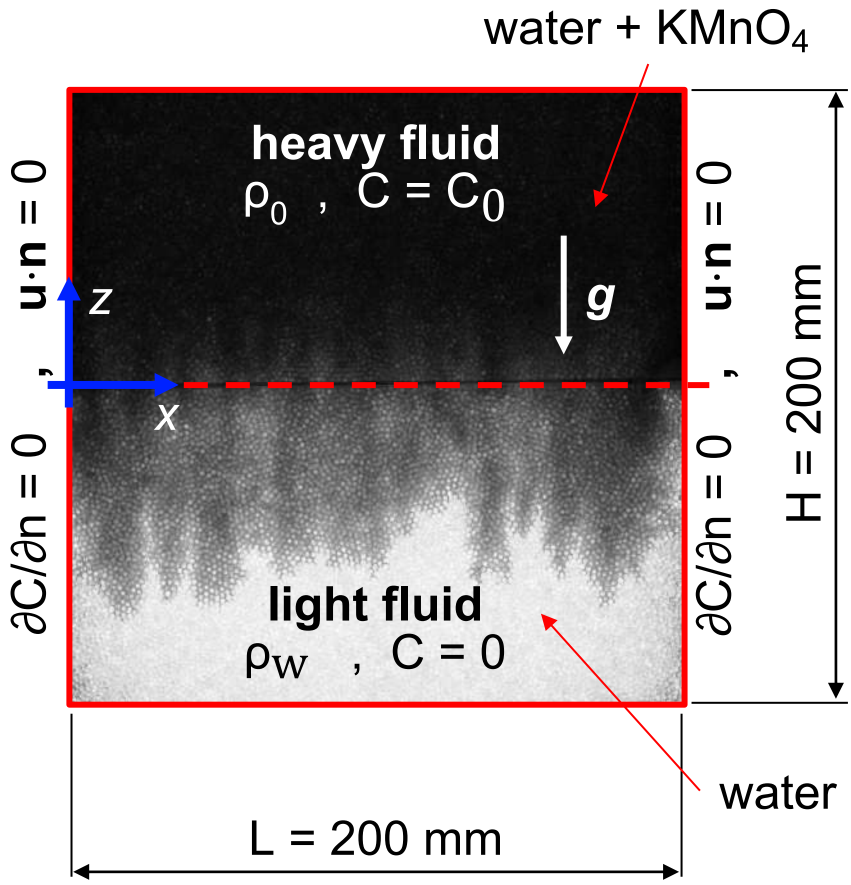
(a) Hele-Shaw cell



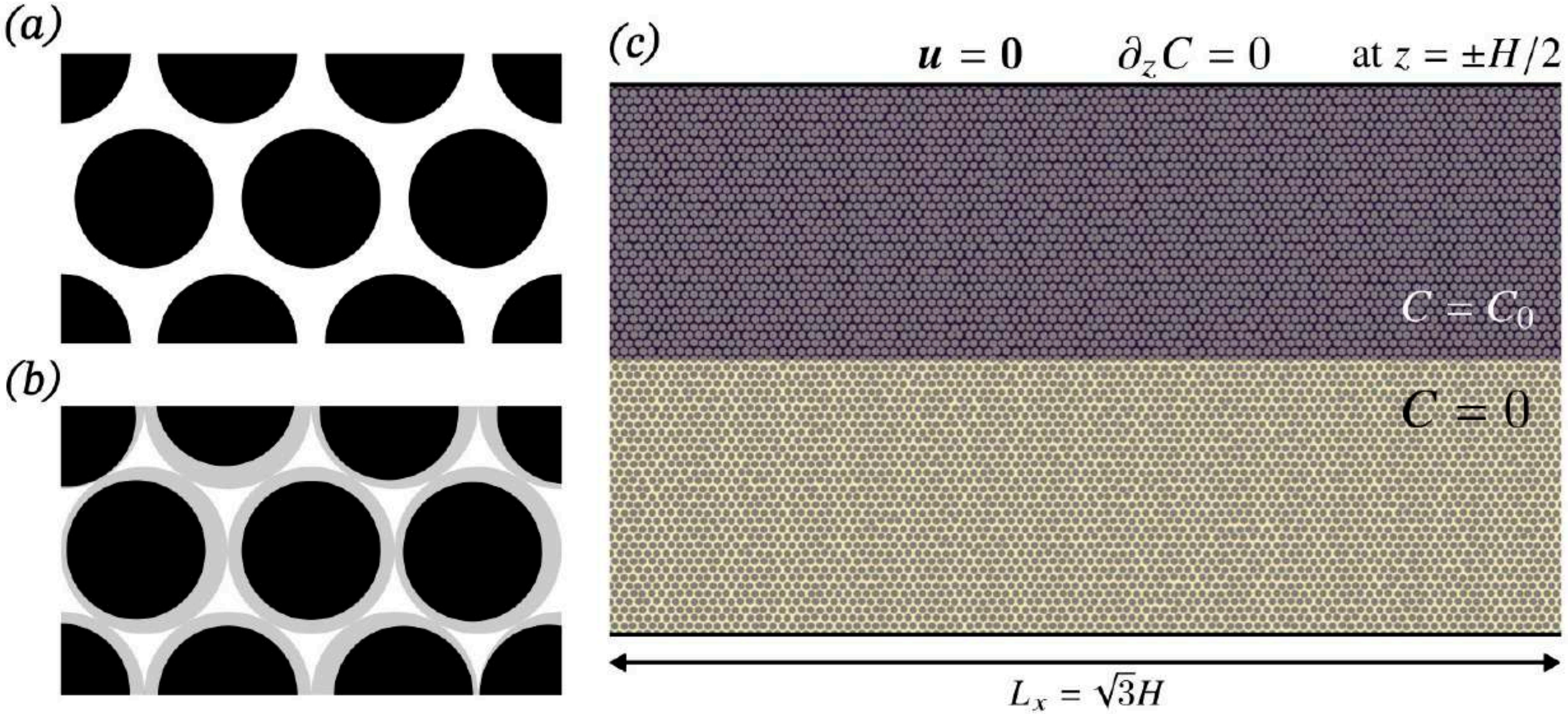
(b) gate (side view)



(c) measurement region



Numerical method



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

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

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

Advanced finite difference (AFiD, open source)
+
Immersed Boundaries Method

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

Characterization of the medium

experiments

Name	H/d	ϕ	Sc	Ra	Ra_d	Ra^*	Pe	Re
E1	200	0.37	558	4.535×10^{10}	5.669×10^{3}	2.173×10^{3}	0.289	0.0005
E2	200	0.37	558	9.099×10^{10}	1.137×10^{4}	4.359×10^{3}	0.580	0.0010
E3	200	0.37	558	1.824×10^{11}	2.280×10^{4}	8.737×10^{3}	1.163	0.0021
E4	200	0.37	558	3.637×10^{11}	4.546×10^{4}	1.742×10^{4}	2.320	0.0042
E5	114	0.37	558	4.667×10^{10}	3.126×10^{4}	6.846×10^{3}	1.595	0.0029
E6	114	0.37	558	9.099×10^{10}	6.096×10^{4}	1.335×10^{4}	3.110	0.0056
E7	114	0.37	558	1.820×10^{11}	1.219×10^{5}	2.671×10^{4}	6.222	0.0112
E8	114	0.37	558	3.626×10^{11}	2.429×10^{5}	5.320×10^{4}	12.395	0.0222
E9	67	0.35	558	4.490×10^{10}	1.515×10^{5}	1.627×10^{4}	5.795	0.0104
E10	67	0.35	558	9.495×10^{10}	3.204×10^{5}	3.441×10^{4}	12.256	0.0220
E11	67	0.35	558	1.834×10^{11}	6.189×10^{5}	6.646×10^{4}	23.672	0.0425
E12	67	0.35	558	3.670×10^{11}	1.239×10^{6}	1.330×10^{5}	47.370	0.0850
E13	50	0.37	558	4.506×10^{10}	3.605×10^{5}	3.454×10^{4}	18.393	0.0330
E14	50	0.37	558	9.101×10^{10}	7.281×10^{5}	6.976×10^{4}	37.150	0.0666
E15	50	0.37	558	1.824×10^{11}	1.460×10^{6}	1.398×10^{5}	74.474	0.1336
E16	50	0.37	558	3.622×10^{11}	2.898×10^{6}	2.777×10^{5}	147.861	0.2652

simulations

Name	H/d	ϕ	Sc	Ra	Ra_d	Ra^*	Pe	Re
S1	17	0.37	100	5.268×10^{8}	1.000×10^{5}	3.334×10^{3}	5.102	0.0510
S2	17	0.37	100	1.666×10^{9}	3.162×10^{5}	1.054×10^{4}	16.135	0.1614
S3	17	0.37	100	5.268×10^{9}	1.000×10^{6}	3.334×10^{4}	51.024	0.5102
S4	35	0.37	100	4.214×10^{9}	1.000×10^{5}	6.669×10^{3}	5.102	0.0510
S5	35	0.37	100	1.333×10^{10}	3.162×10^{5}	2.109×10^{4}	16.135	0.1614
S6	35	0.37	100	4.214×10^{10}	1.000×10^{6}	6.669×10^{4}	51.024	0.5102
S7	52	0.37	100	1.422×10^{10}	1.000×10^{5}	1.000×10^{4}	5.102	0.0510
S8	52	0.37	100	4.498×10^{10}	3.162×10^{5}	3.163×10^{4}	16.135	0.1614
S9	52	0.37	100	1.422×10^{11}	1.000×10^{6}	1.000×10^{5}	51.024	0.5102
S10	70	0.37	100	3.372×10^{10}	1.000×10^{5}	1.334×10^{4}	5.102	0.0510
S11	70	0.37	100	1.066×10^{11}	3.162×10^{5}	4.218×10^{4}	16.135	0.1614
S12	70	0.37	100	3.372×10^{11}	1.000×10^{6}	1.334×10^{5}	51.024	0.5102

dimensionless parameters

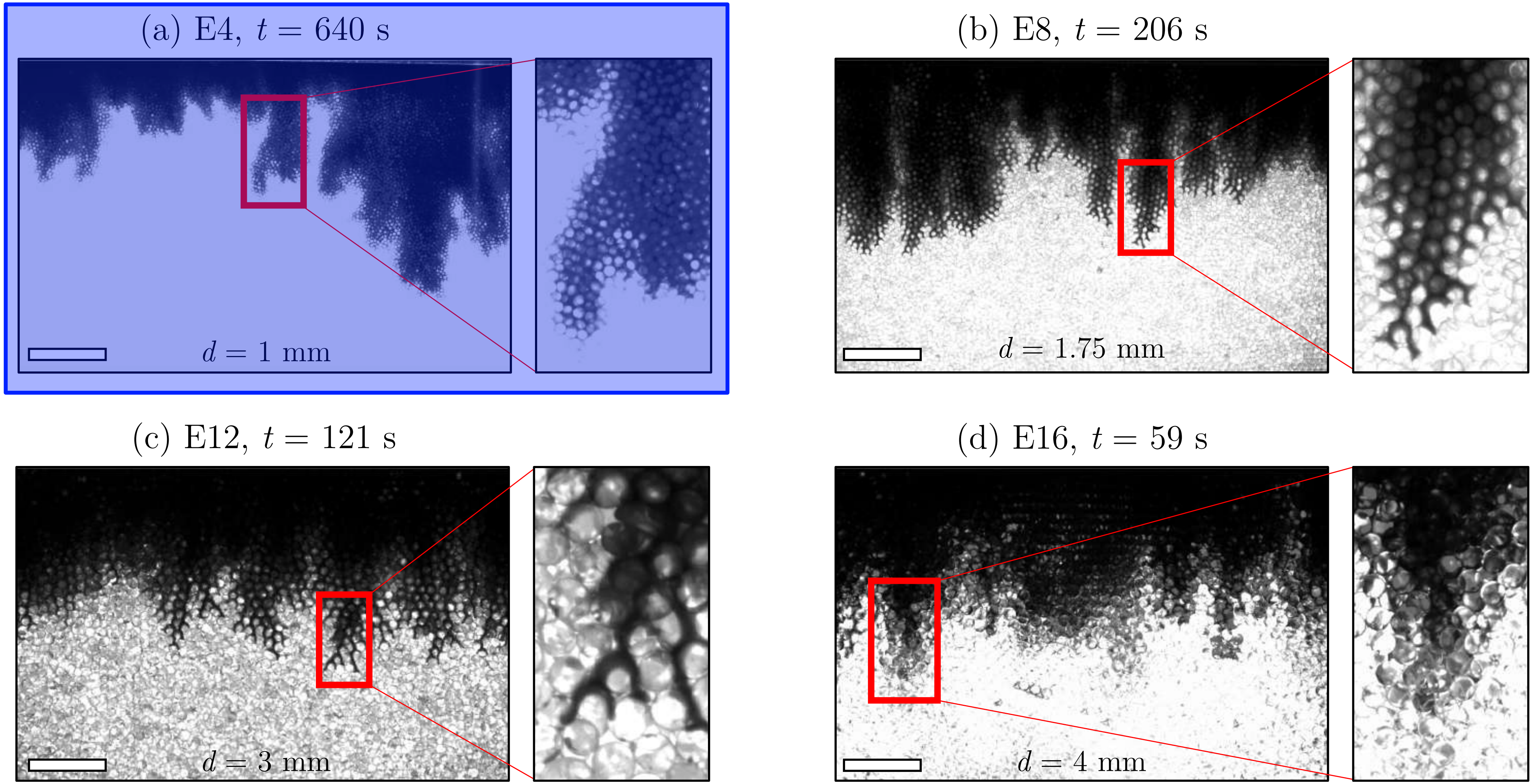
$$Da = k/H^2 \qquad Ra = \frac{g\Delta\rho H^3}{\mu D} \qquad Ra_d = \frac{g\Delta\rho d^3}{\mu D}$$

$$Ra^* = \frac{Ra\,Da}{\phi} \qquad Re = \frac{Ra^*\,Da^{1/2}}{Sc} \qquad Pe = Ra^*\,Da^{1/2}$$

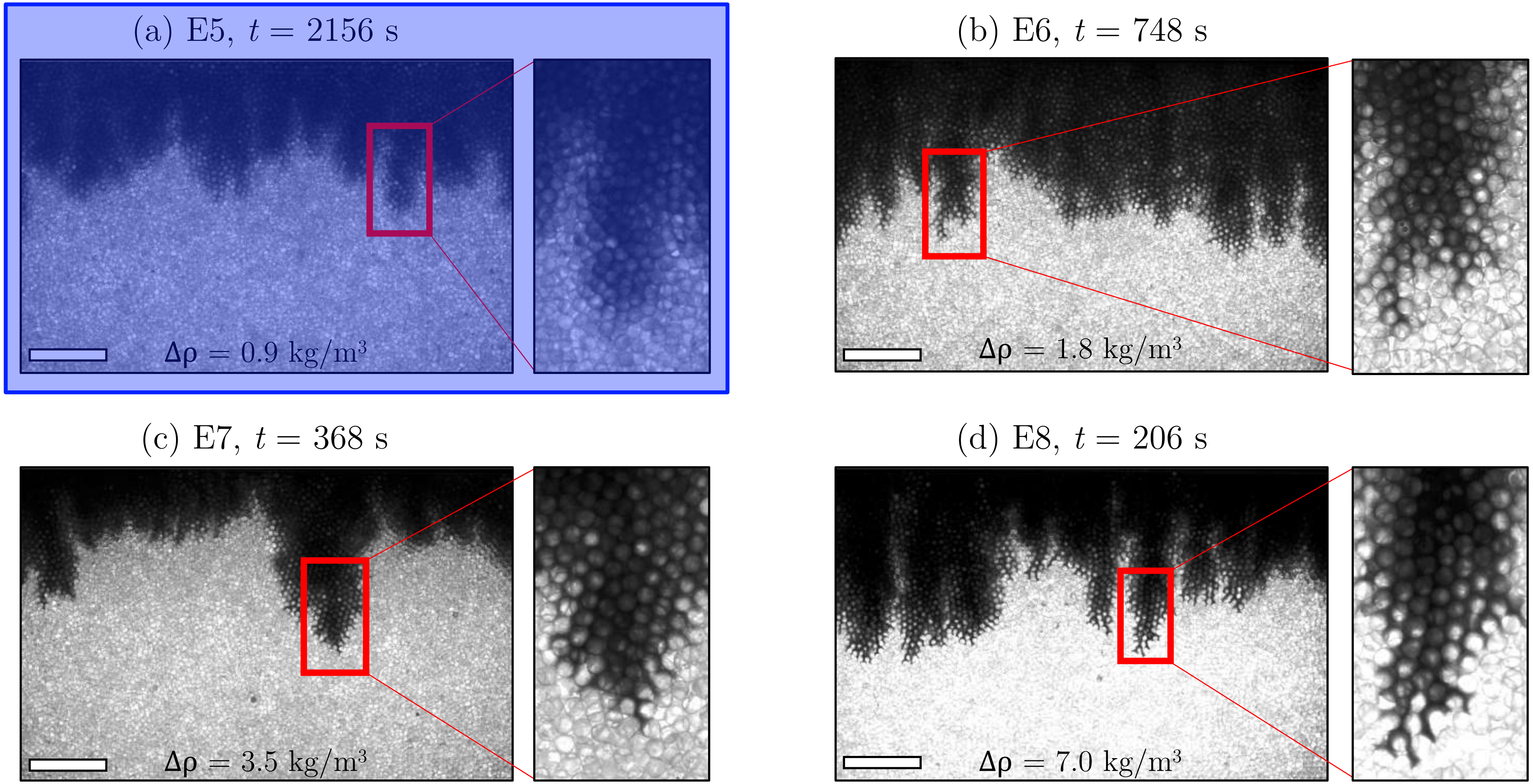
flow scales and parameters

$$k = \frac{d^2}{36k_C}\frac{\phi^3}{(1-\phi)^2} \qquad U = \frac{g\Delta\rho k}{\mu} \qquad \ell = \frac{\phi D}{U} \qquad Sc = \frac{\mu}{\rho_0 D}$$

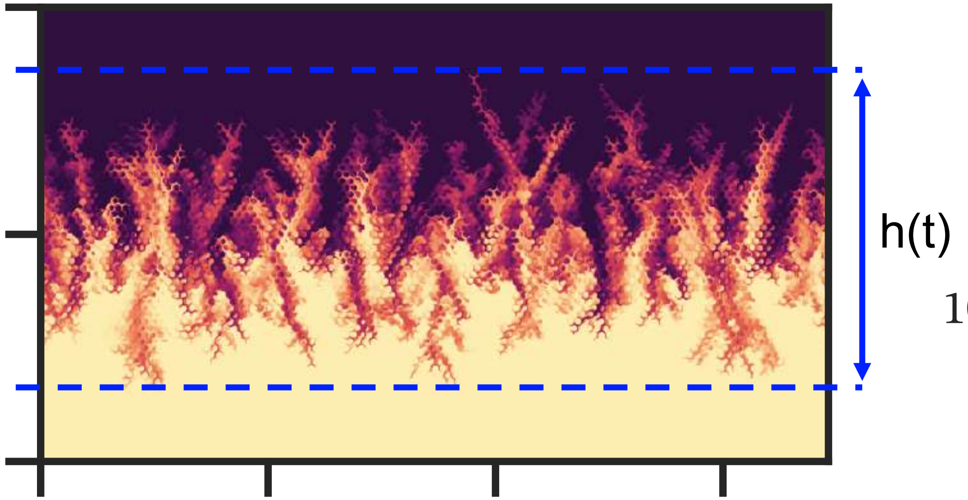
Influence of d ($\Delta\rho$ = 7 kg/m^3)



Influence of Δρ (d = 1.75 mm)



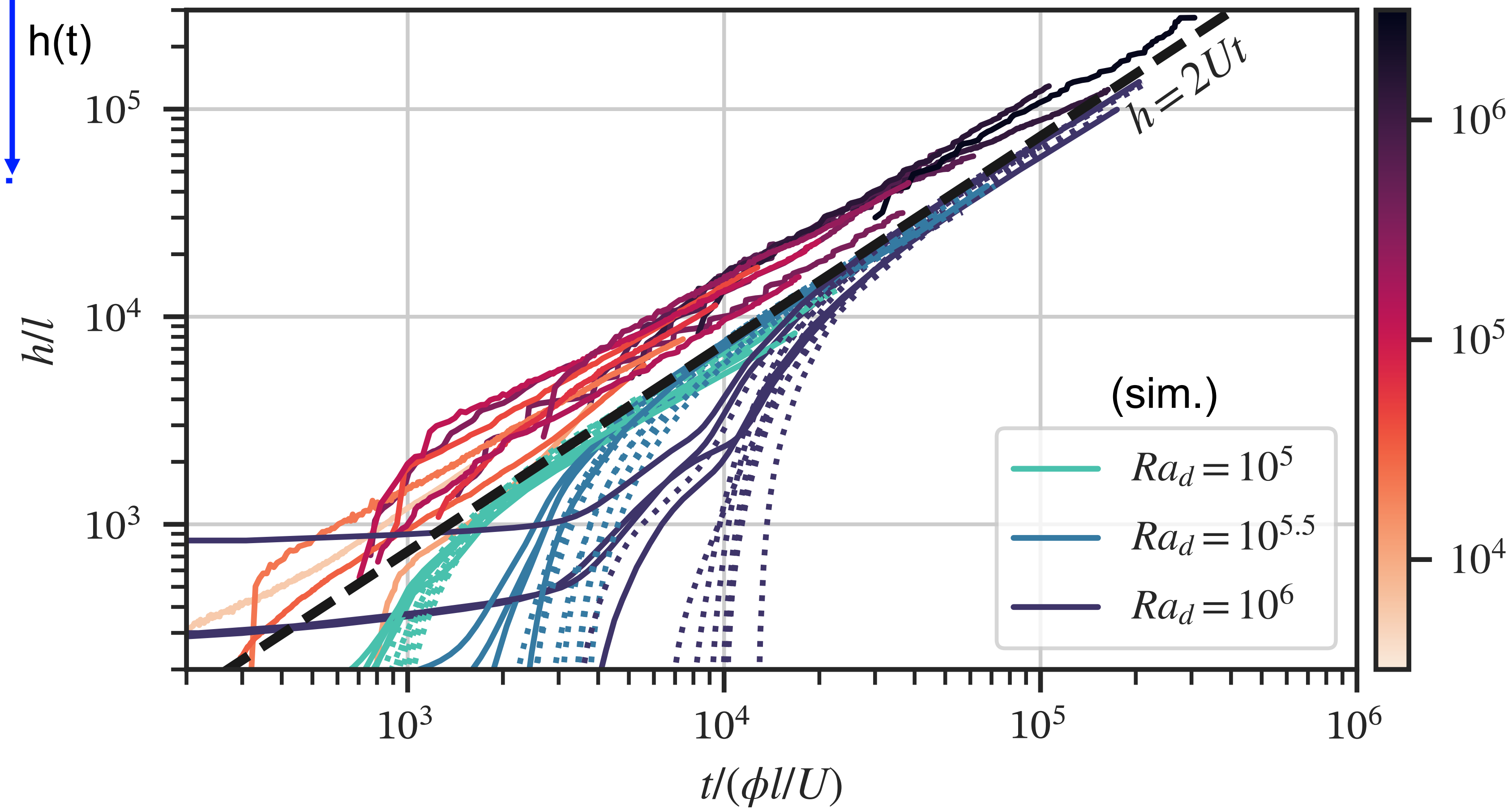
Mixing length



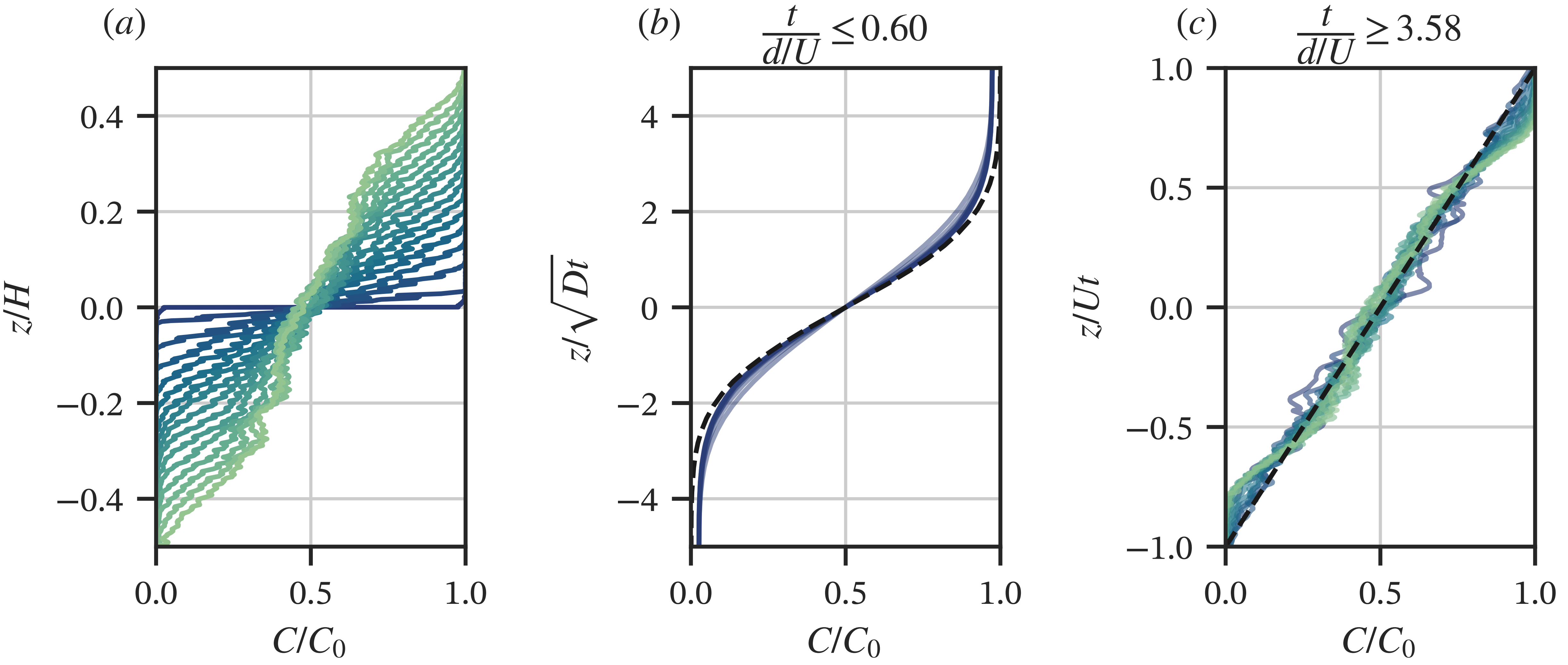
$$U = \frac{g\Delta\rho k}{\mu}$$

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

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



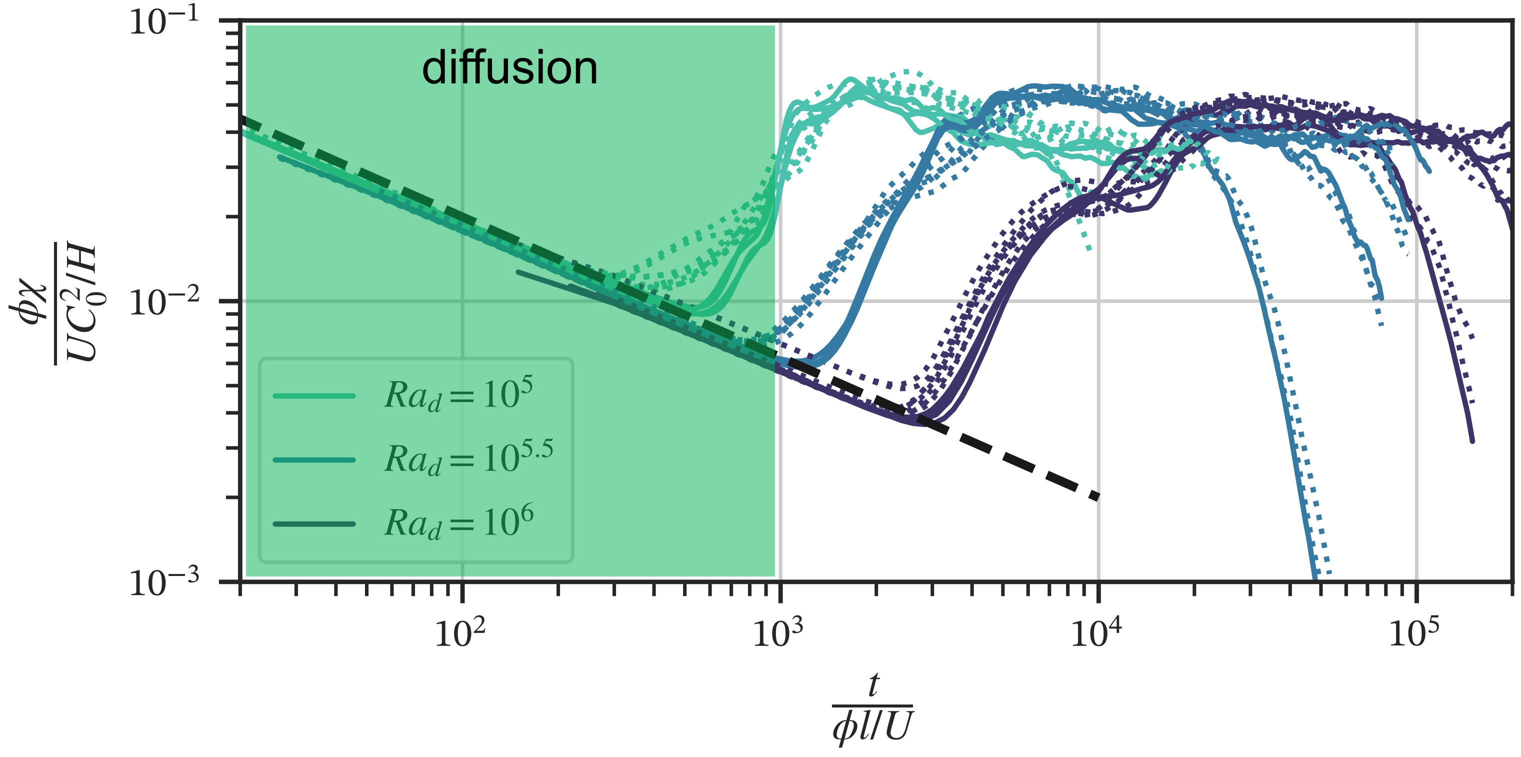
Concentration profiles



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:

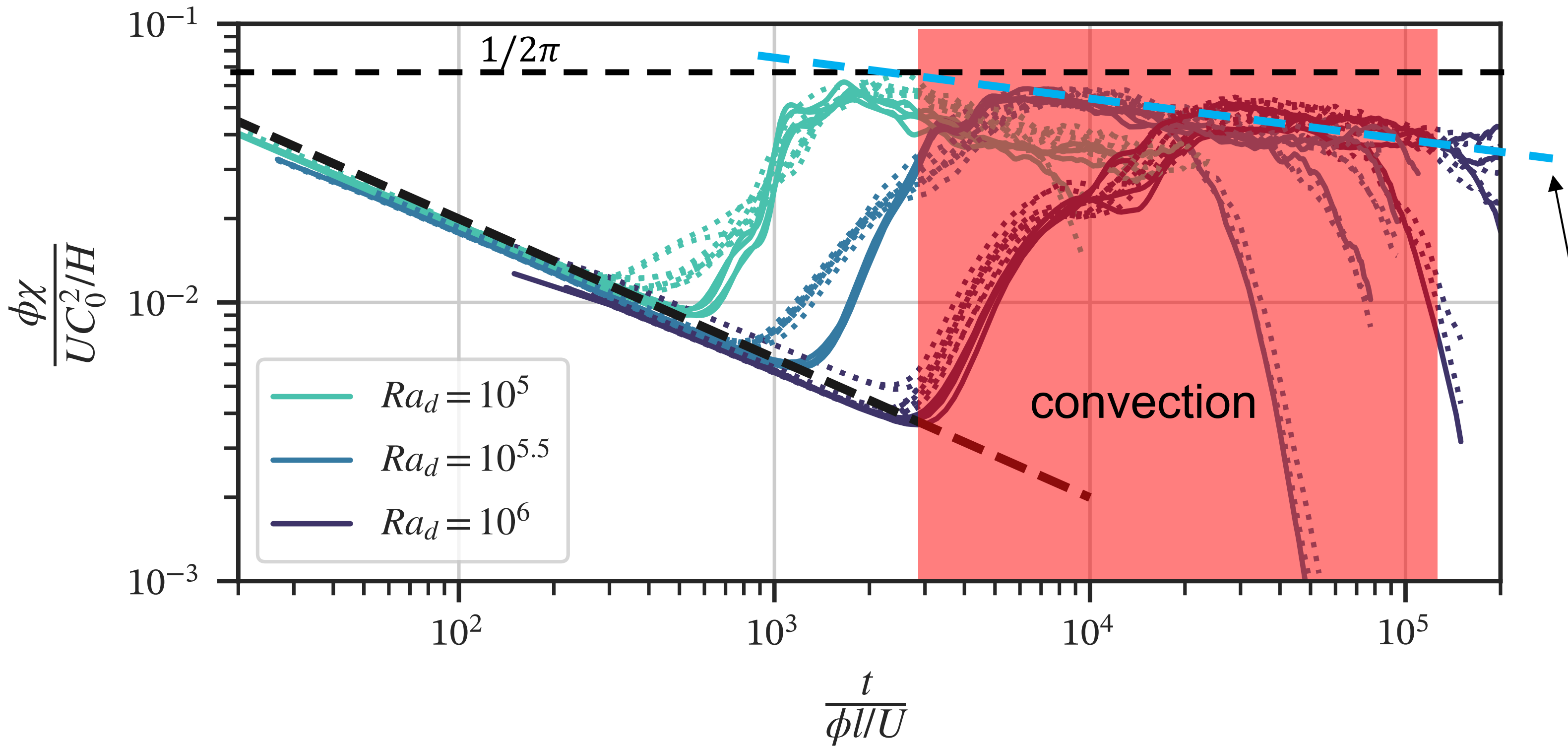
$$C = C_0 + \frac{\Delta C}{2}\mathrm{erf}\left(\frac{z}{\sqrt{2\kappa t}}\right)$$

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

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

Modelling scalar dissipation

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



Convection

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

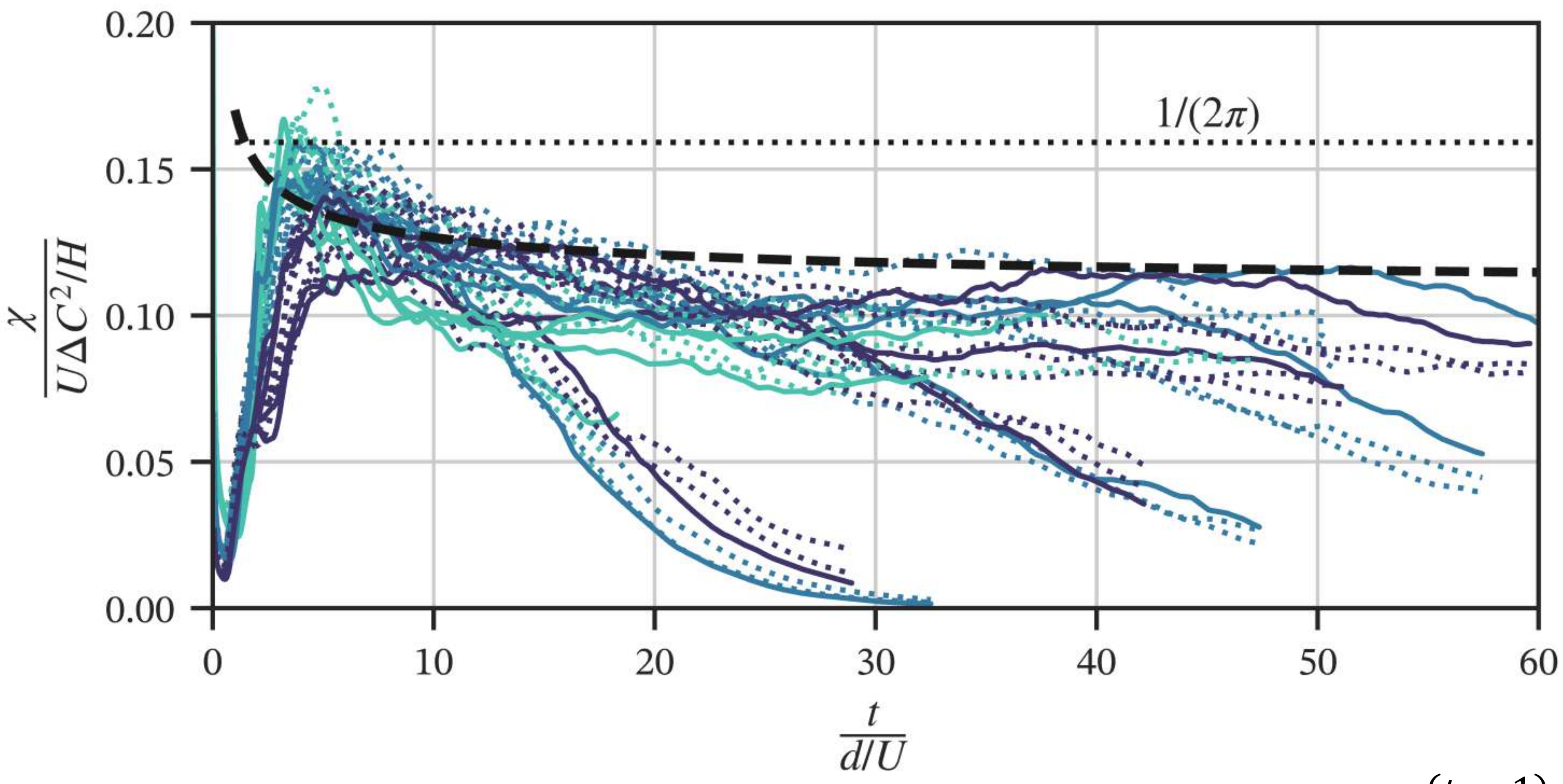
$$|\nabla C| \approx \frac{\Delta C}{2\sqrt{\pi\kappa t}}.$$

$$L_m \approx 2Ut,$$

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

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

Modelling scalar dissipation

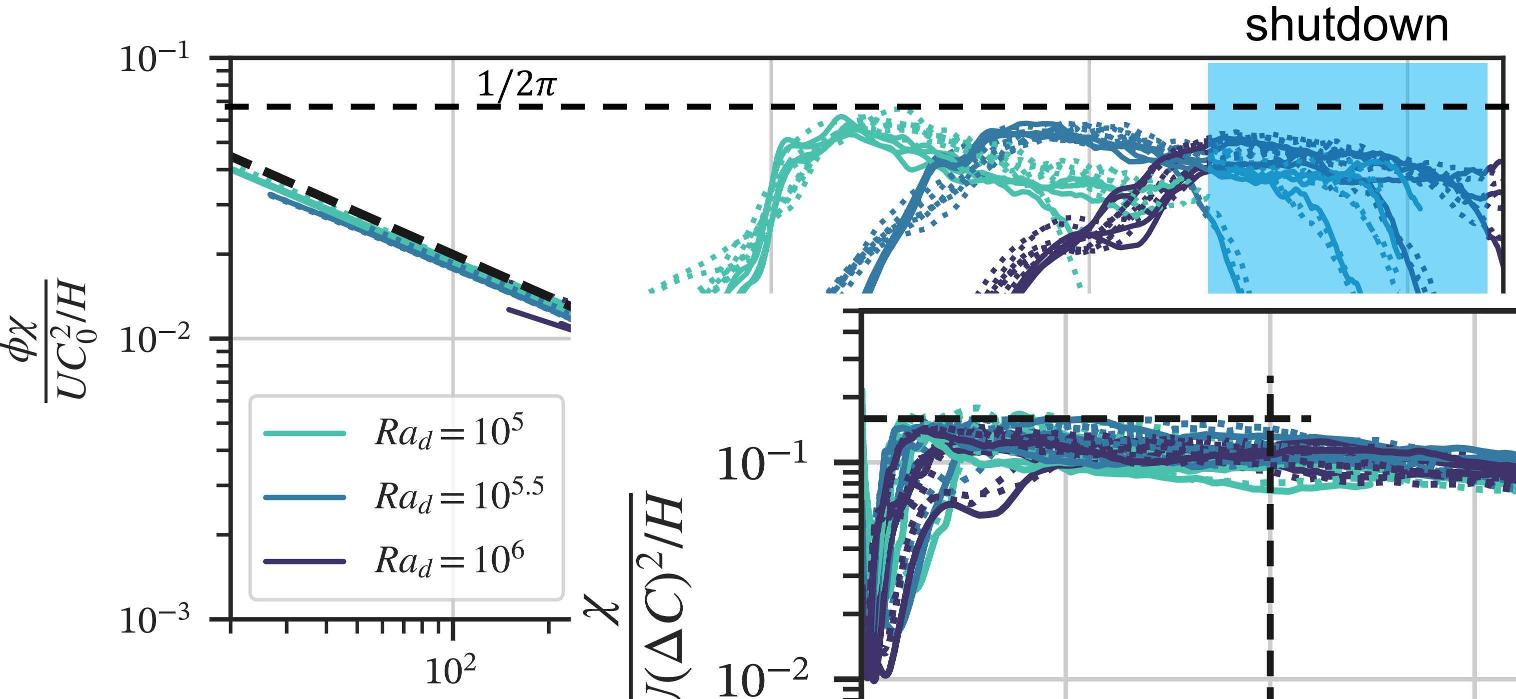


$1/2\pi$ is the maximum value of dissipation.

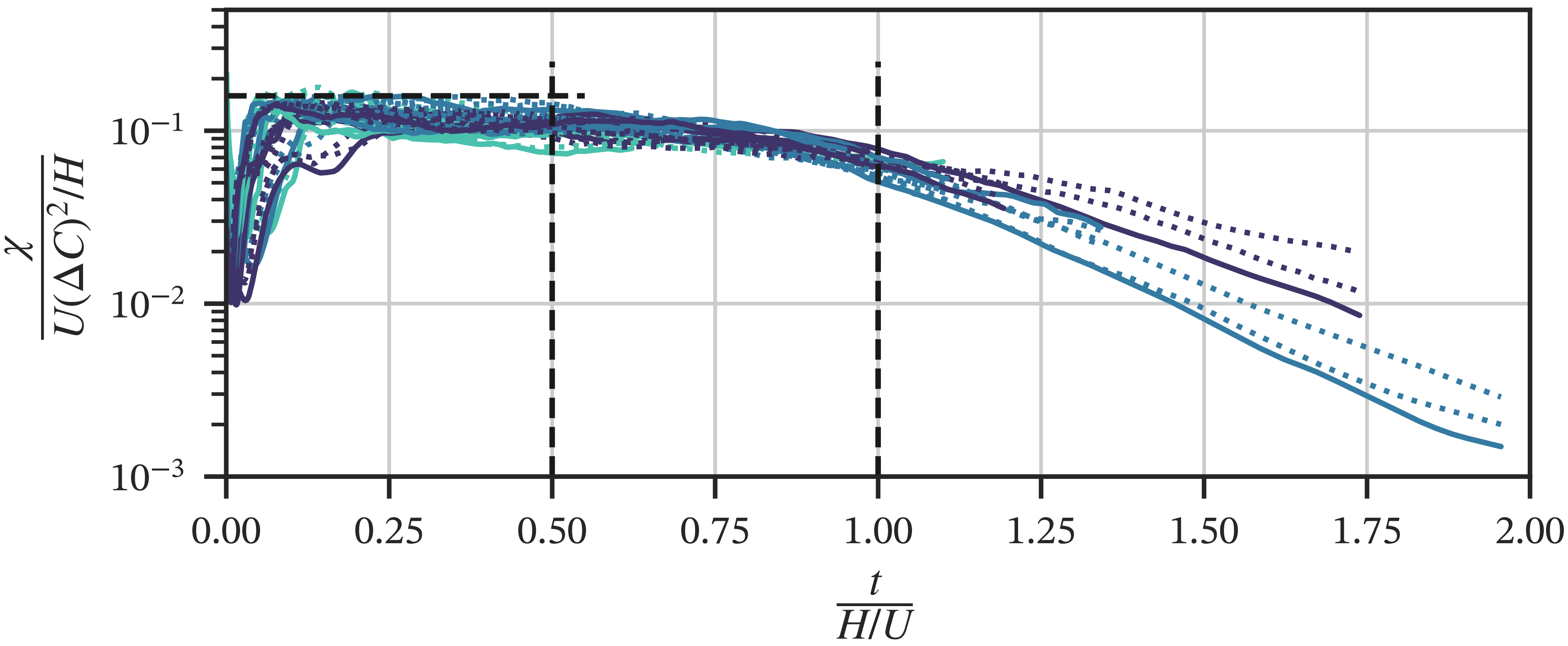
Model shown starting from $t/(d/U)$ =1. Time is also increased by d/U to account for initial condition.

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

Modelling scalar dissipation



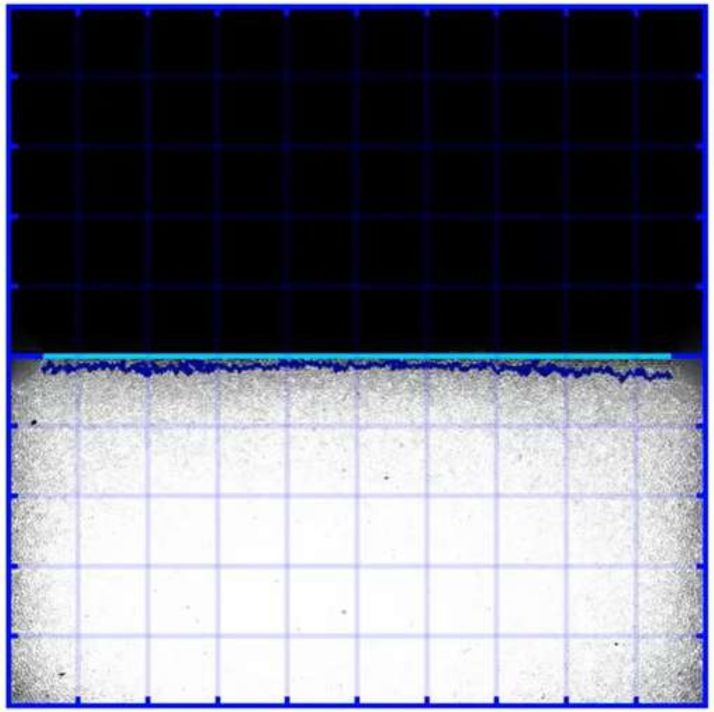
$$Ra^* = \frac{g\Delta\rho k H}{\mu\phi D} = \frac{UH}{\phi D} = \frac{H}{\ell} = \frac{Ra\,Da}{\phi}$$

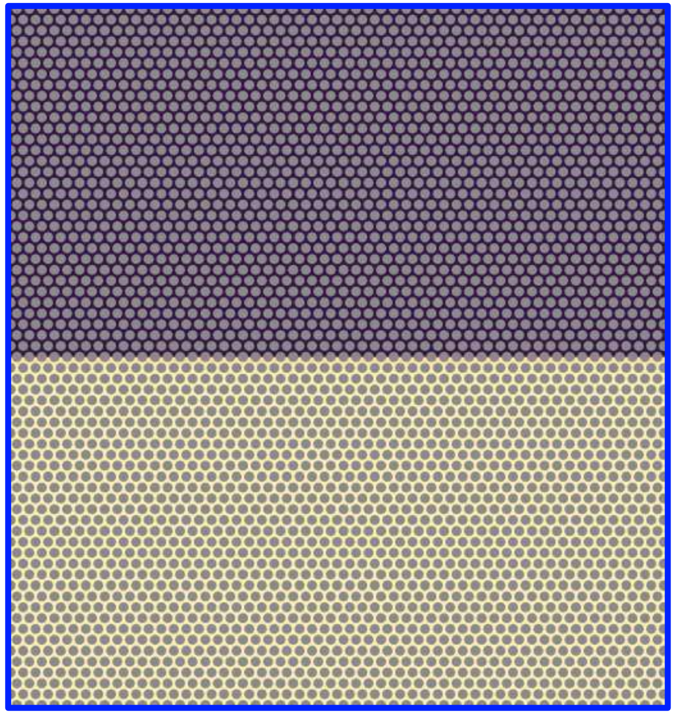


$$\ell = \frac{\phi D}{U}$$

Conclusions

- Simulations and experiments are used as complementary tools to investigate convection in porous media
- Multiple length scales are relevant at different phases of the process
- Mixing length predicted experimentally exhibits a self-similar behaviour that agrees well with theoretical prediction for convective flows in porous media
- Mixing measured numerically via mean scalar dissipation has a self-similar behaviour.
- We explain theoretically the scaling laws observed
- We plan to expand the parameters space investigated and performed simulations in three-dimensional domains





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Der Wissenschaftsfonds.

Thank you for your attention! Questions?

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