Multiscale modelling of convection in porous media:

experiments, pore-scale and Darcy simulations with dispersion

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)

Acknowledgements

UNIVERSITY OF TWENTE.

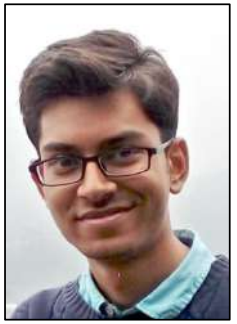
Physics of Fluids

MAX-PLANCK-GESELLSCHAFT

D. Lohse

C. Howland

G. Yerragolam



R. Verzicco

G S S I Università di Roma Tor Vergata

TU WIEN

This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Sklodowska-Curie grant agreement MEDIA No. 101062123.

European Commission

Marie Skłodowska-Curie Actions

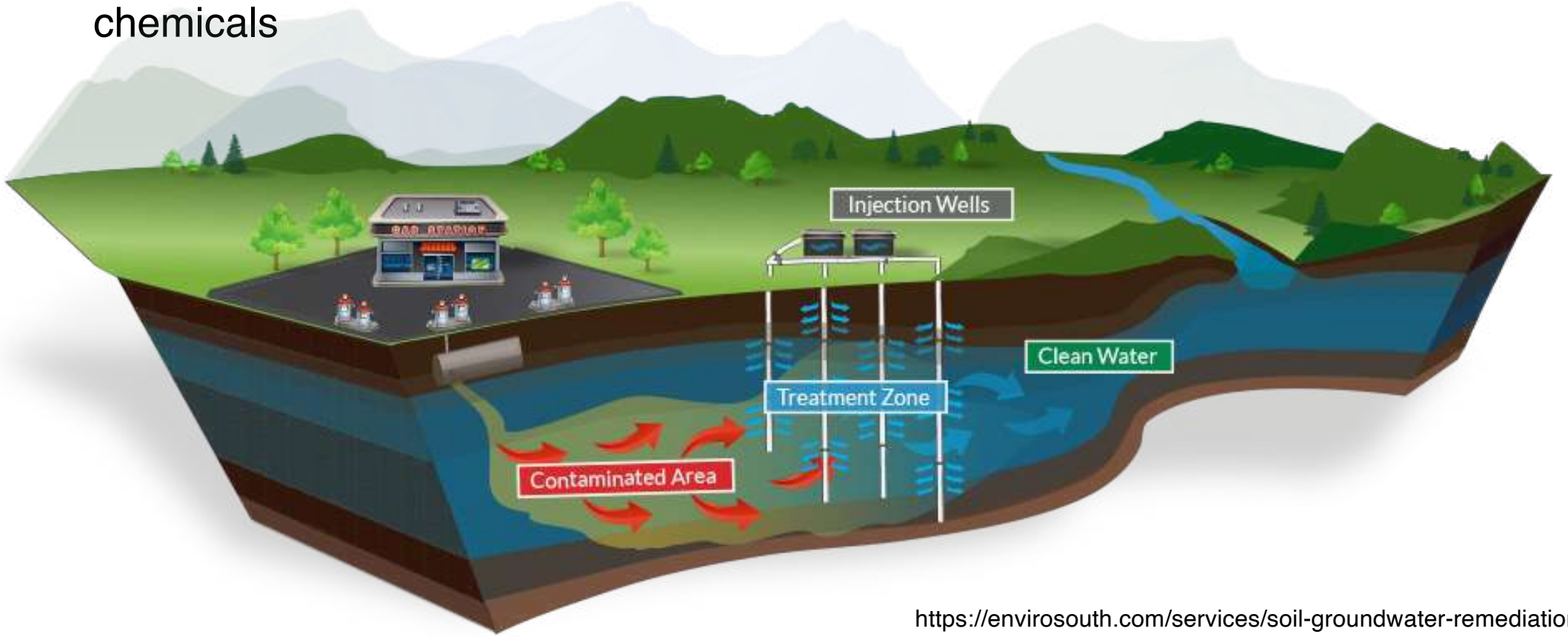
MAX-PLANCK-GESELLSCHAFT

SURF

EuroHPC Joint Undertaking

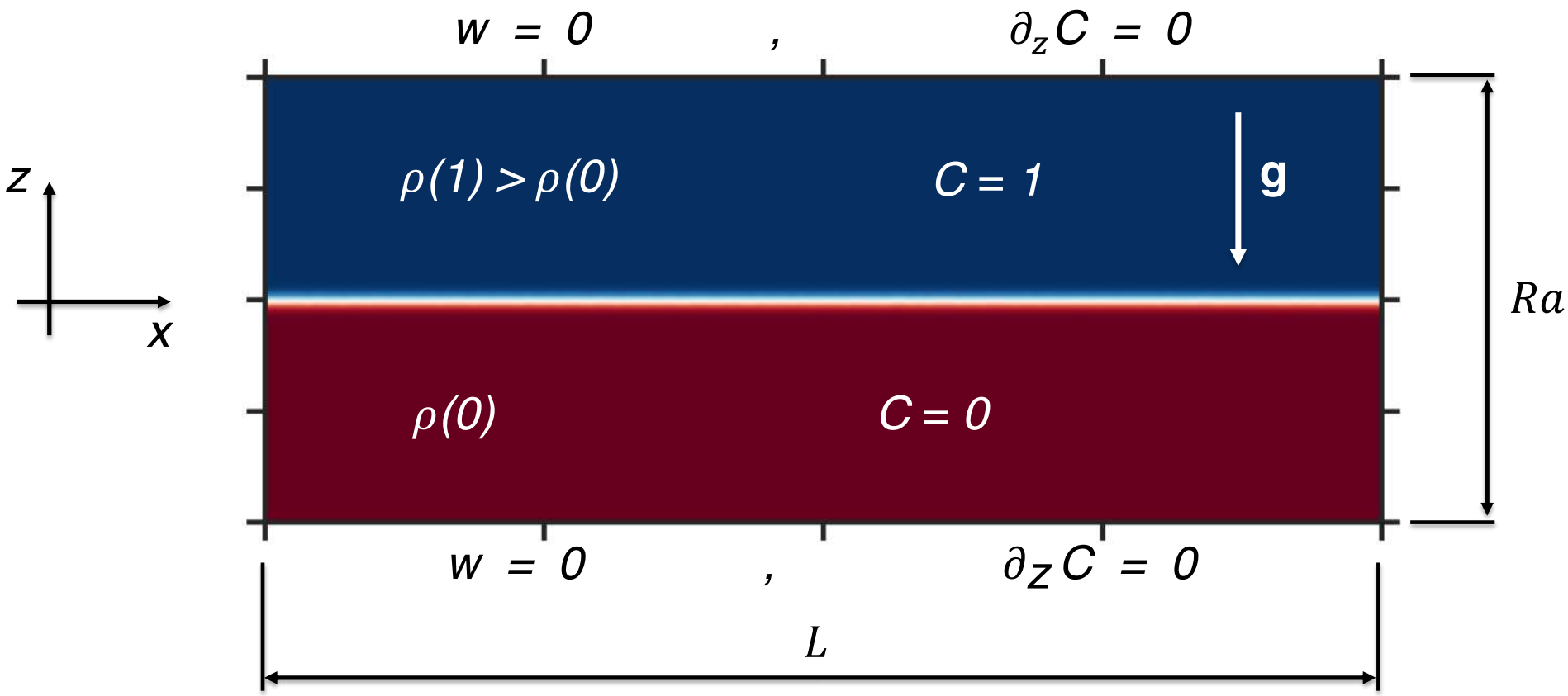
Funded by the European Union

Groundwater remediation, e.g., of light and dense non-aqueous petroleum liquids (LNAPL, DNAPL), resulting from spillage of fuels or chemicals

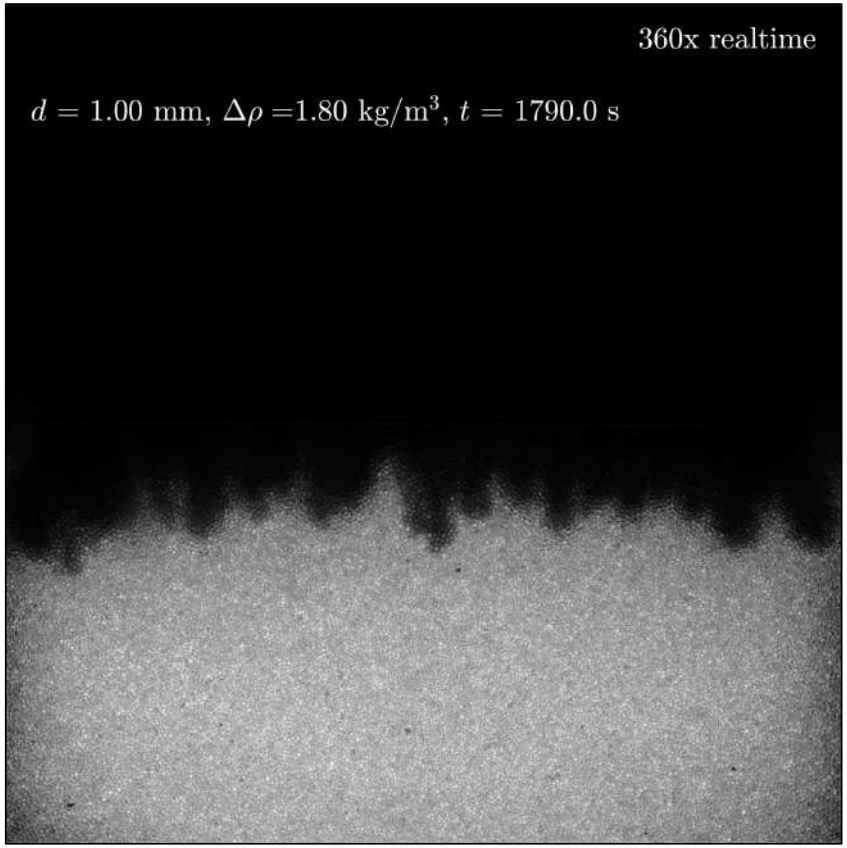


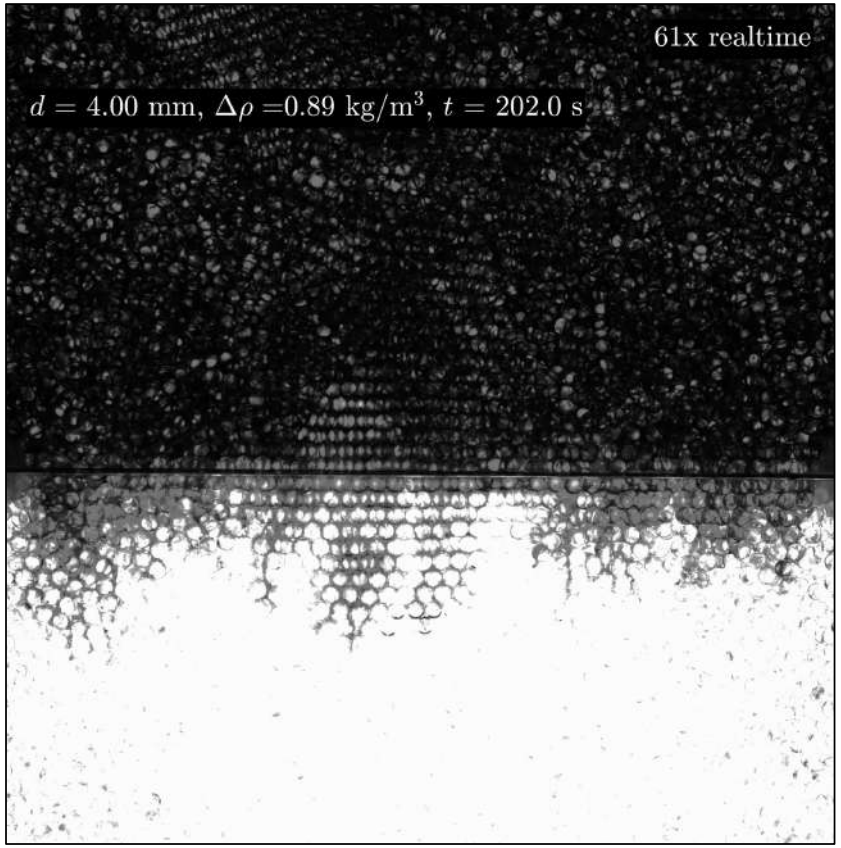
https://envirosouth.com/services/soil-groundwater-remediation/

Flow configuration



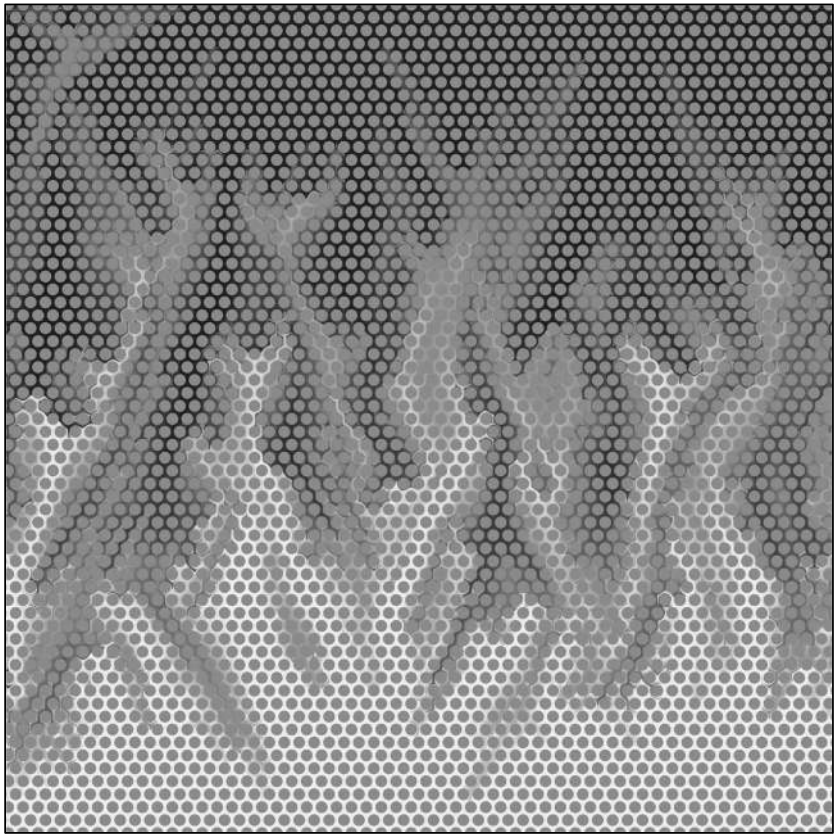
Experiments





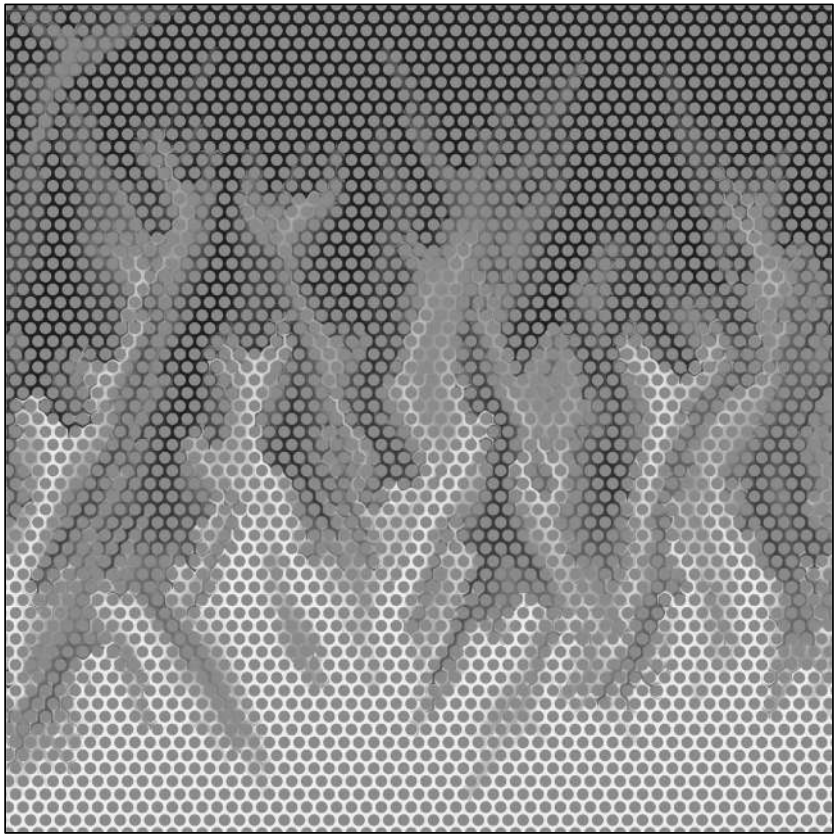
De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D. (2024). *Journal of Fluid Mechanics*, *987*, A1.

pore-scale

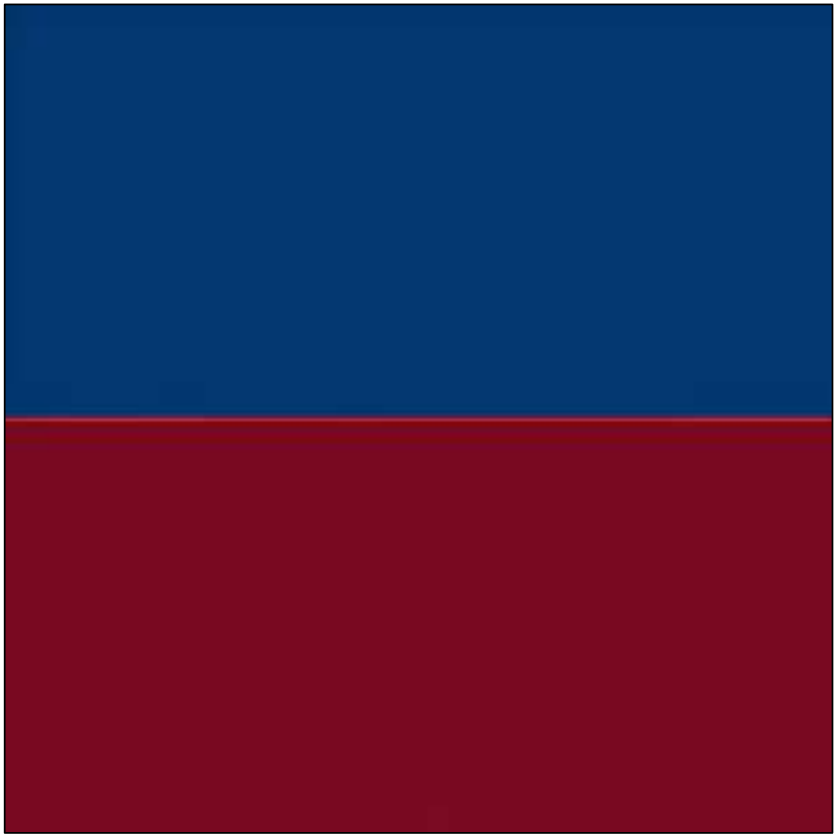


De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D. (2024). *Journal of Fluid Mechanics*, *987*, A1.

pore-scale



Darcy scale



De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D. (2024). *Journal of Fluid Mechanics*, *987*, A1.

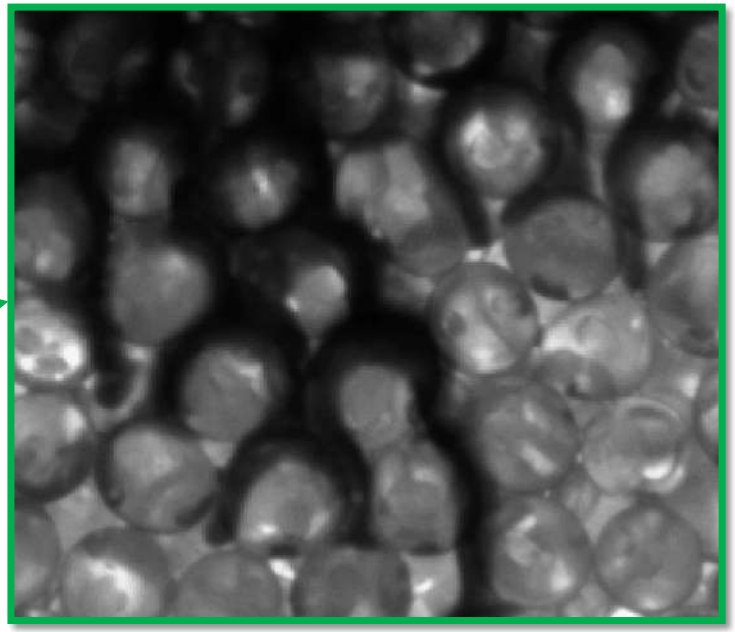
Governing equations

$$\nabla \cdot \mathbf{u} = 0 \qquad \mathbf{u} = -(\nabla p + C\mathbf{k})$$

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

$$\boldsymbol{D}^* = D_m^* \boldsymbol{I} + (\alpha_l^* - \alpha_t^*) \frac{\mathbf{u}^* (\mathbf{u}^*)^{\mathrm{T}}}{|\mathbf{u}^*|} + \alpha_t^* \boldsymbol{I} |\mathbf{u}^*|$$

$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta} \left[(r-1) \frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I} |\mathbf{u}| \right]$$



convection

$$Ra = \frac{g \Delta \rho^* K L_z^*}{\phi D_m^* \mu} = \frac{\mathscr{U}^* L_z^*}{\phi D_m^*}$$

Bear, *J. Geophys. Res.* (1961)
Wen, Chang & Hesse, *Phys. Rev. Fluids* (2018)

dispersion

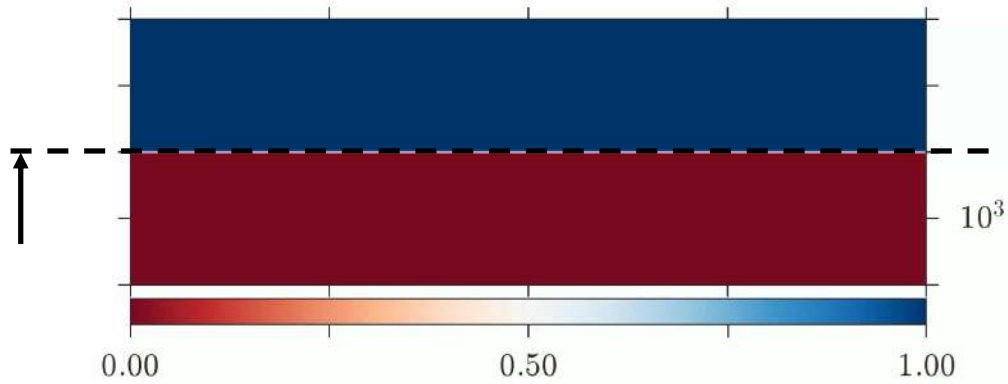
$$\Delta = \frac{D_m^*}{D_t^*} \quad , \quad r = \frac{D_l^*}{D_t^*} = \frac{\alpha_l^*}{\alpha_t^*}$$

De Paoli, Yerragolam, Lohse & Verzicco, **AFiD-Darcy**, *Comput. Phys. Comm.* (2025) (*code open sourced*)

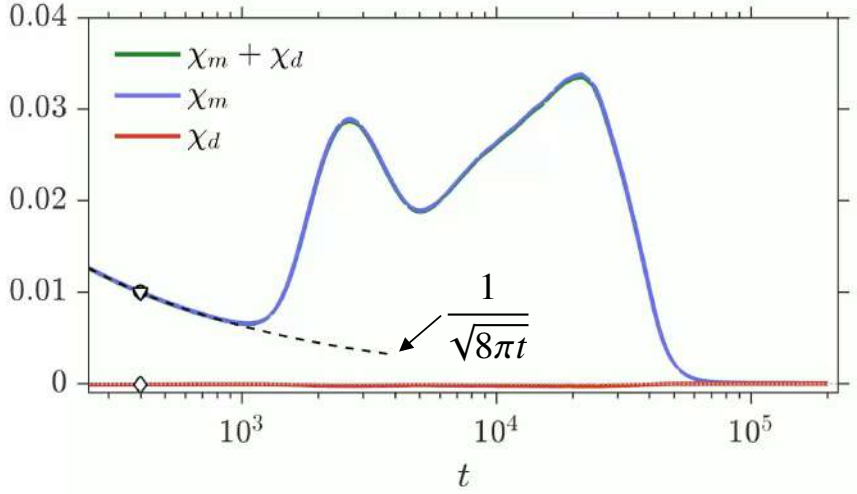
No dispersion ($\Delta \to \infty$)

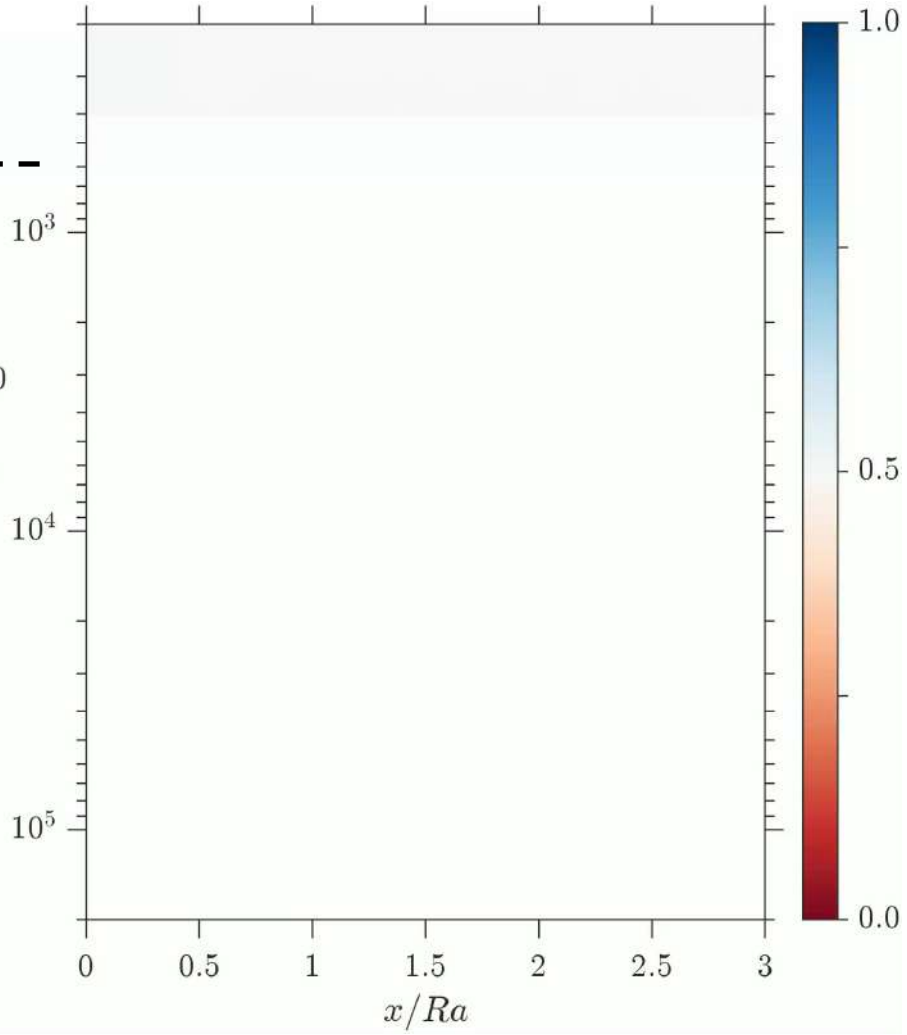
$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

InterPore

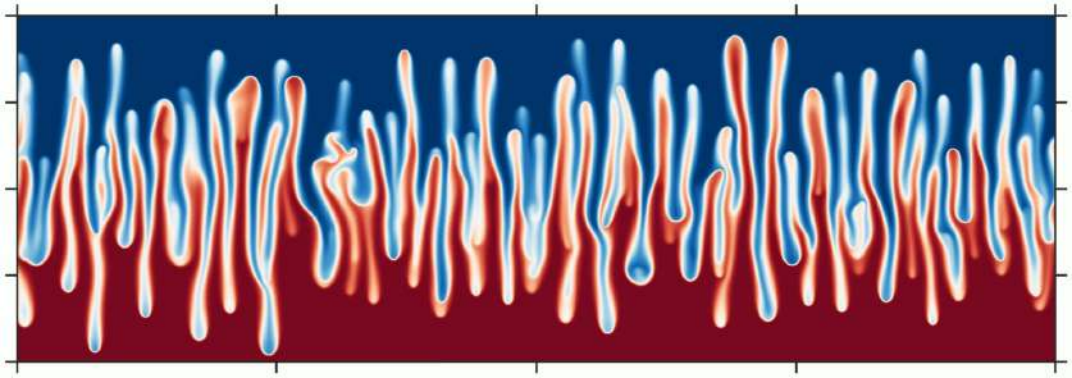


$$\chi_m = Ra\langle|\nabla C|^2\rangle, \quad \chi_d = Ra\langle(\nabla C)\cdot(\boldsymbol{D}\nabla C) - |\nabla C|^2\rangle$$

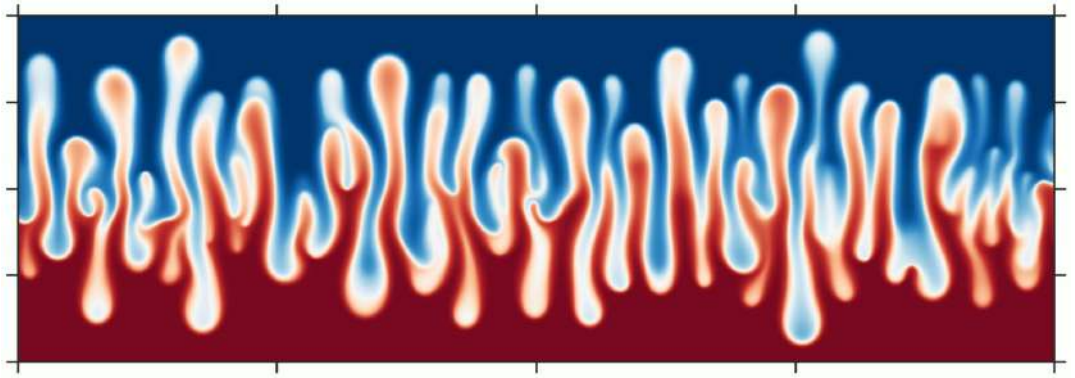




variable $r, \Delta = 0.1, \mathrm{Ra} = 10^4$



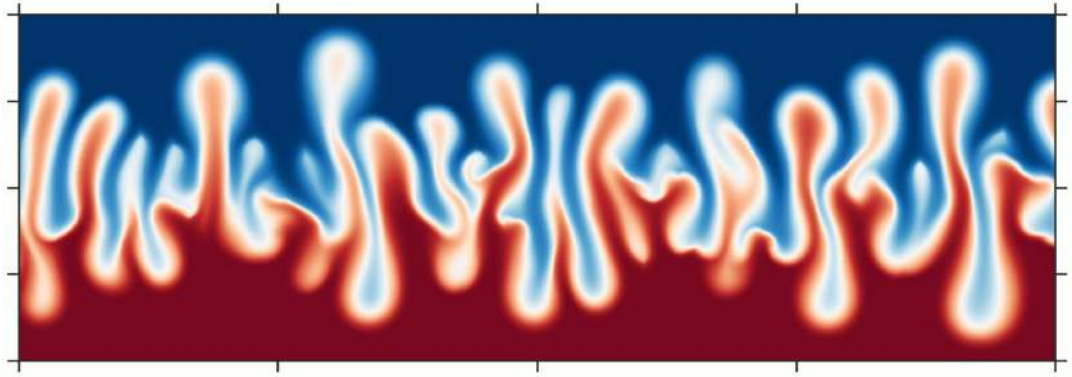
No dispersion



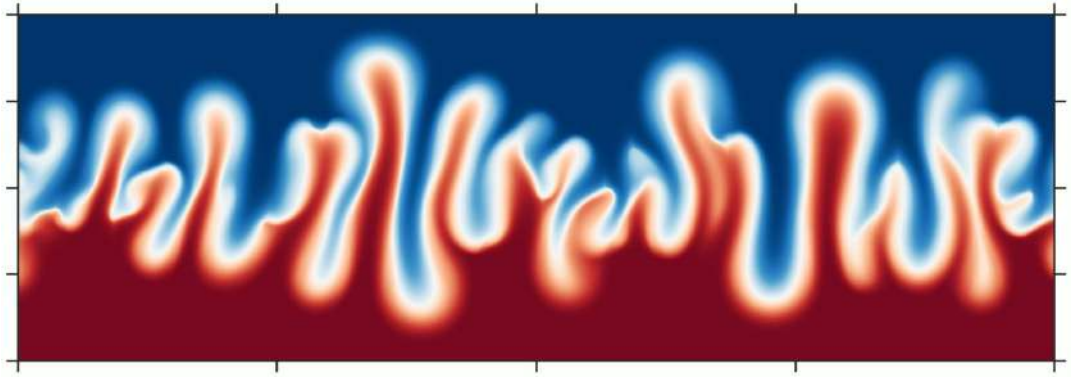
$r = 1$

$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

$r = 10$

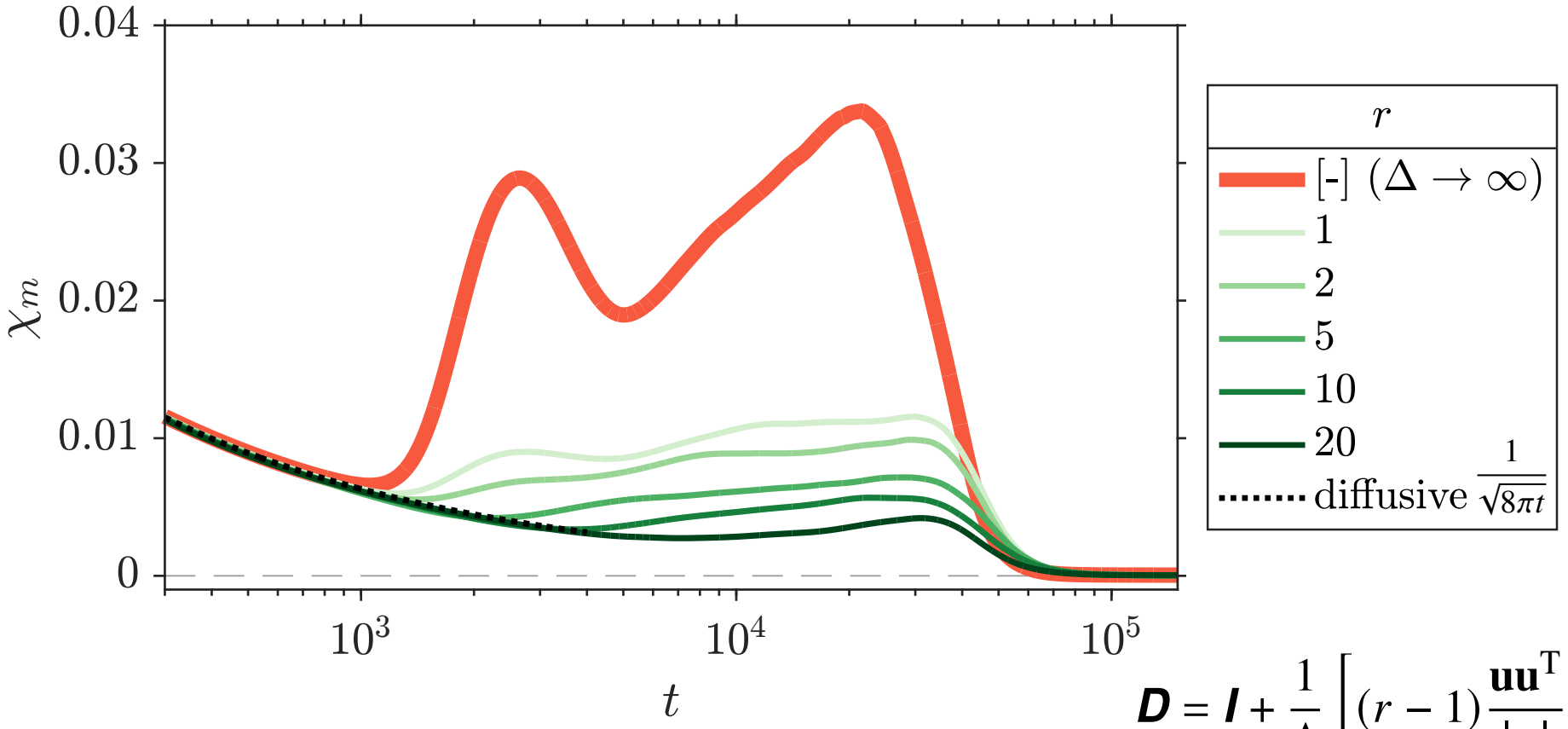


$r = 20$



Molecular dissipation

$$\chi_m = Ra\langle|\nabla C|^2\rangle$$

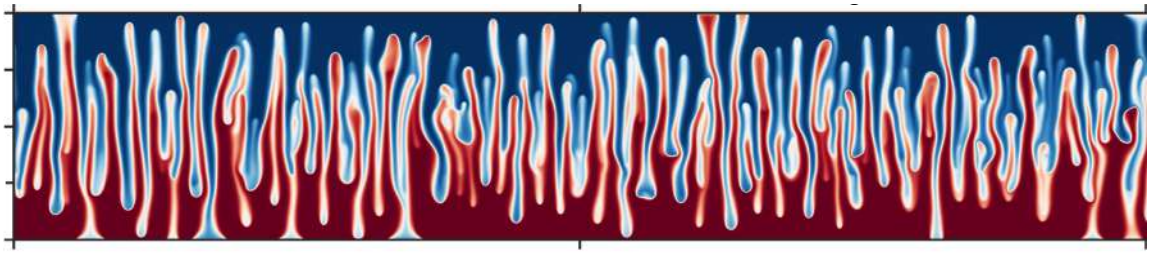


$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

Molecular dissipation

(a)

No dispersion

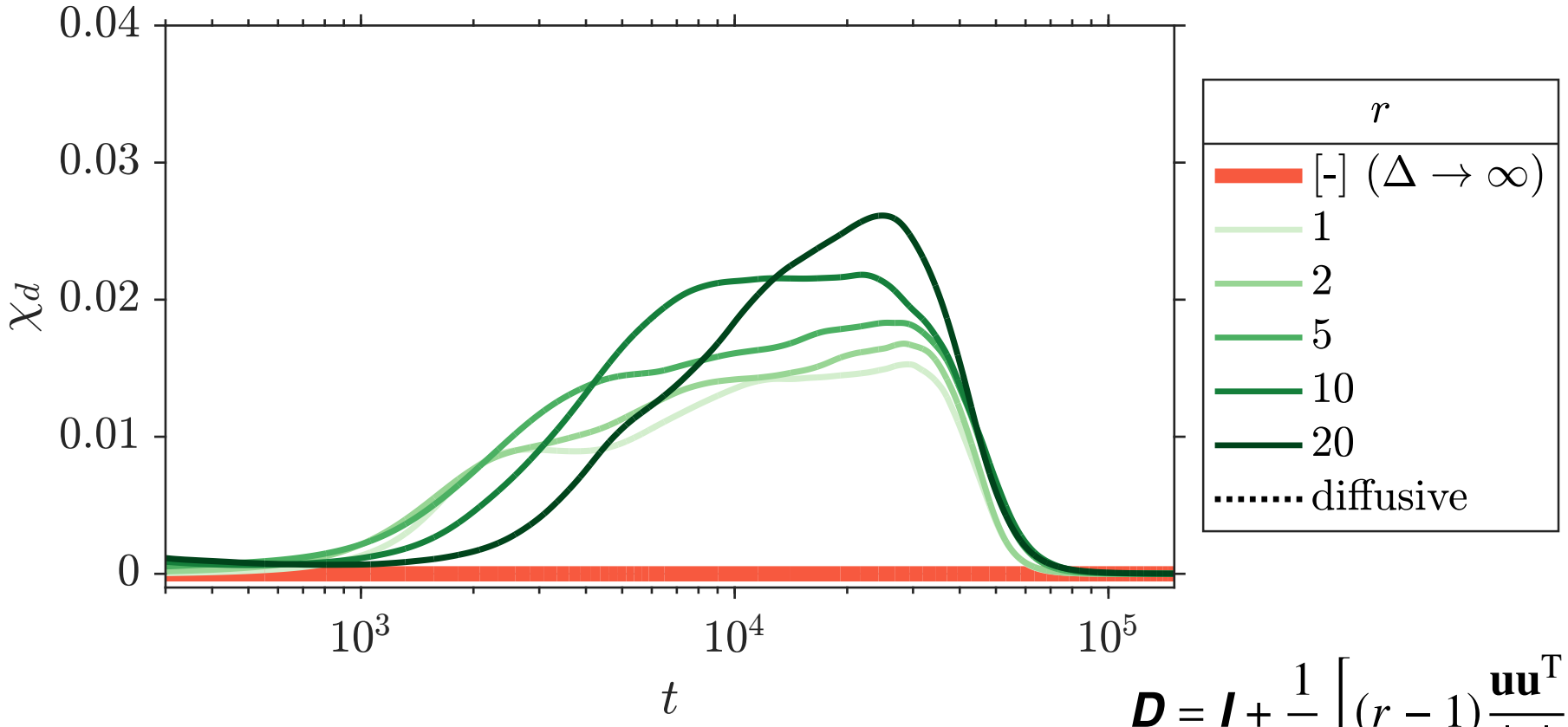


$$\chi_m = Ra\langle|\nabla C|^2\rangle$$

Gradient across the interface of the fingers reduces

Dispersive dissipation

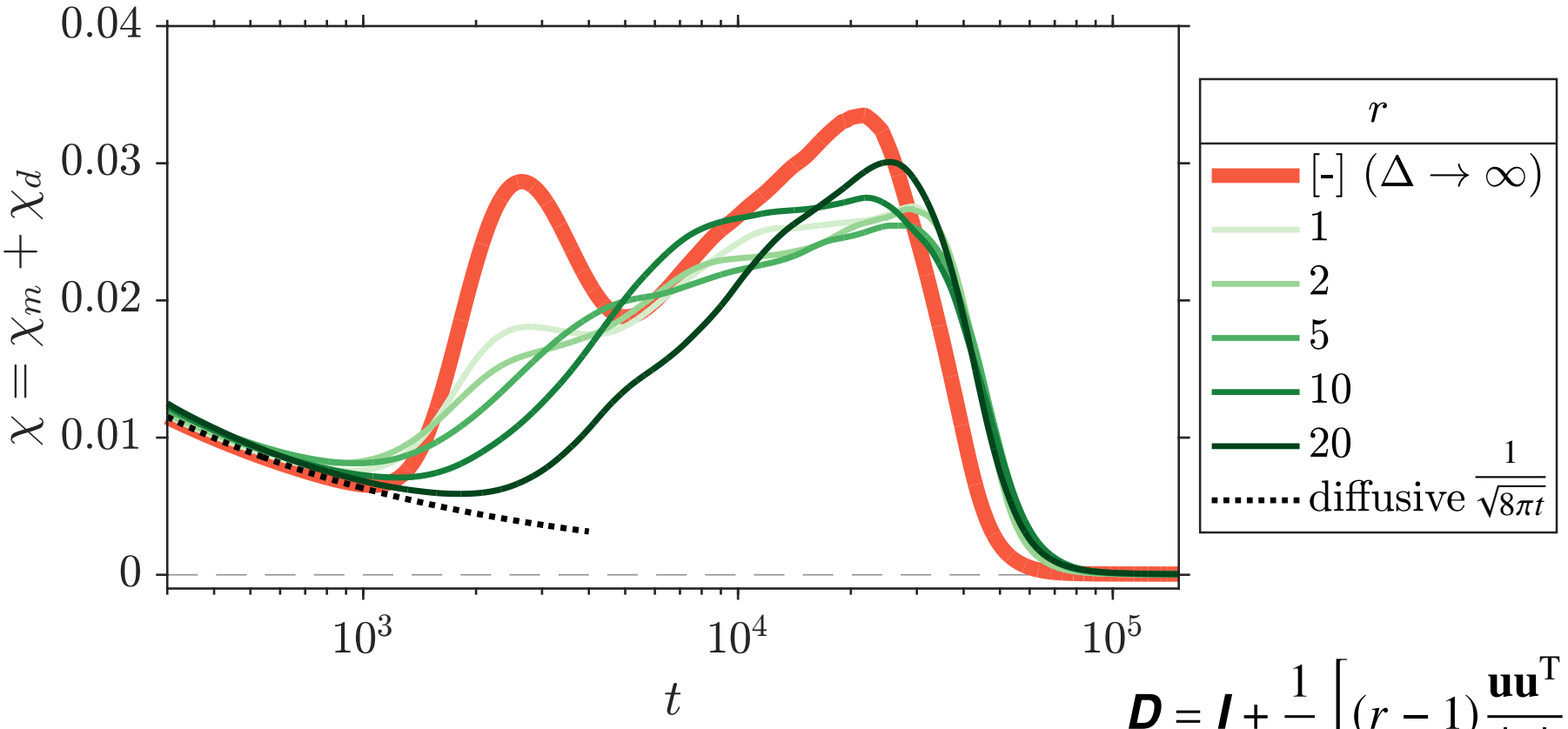
$$\chi_d = Ra\langle(\nabla C)\cdot(\boldsymbol{D}\nabla C) - |\nabla C|^2\rangle$$



$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

Total dissipation

$$\chi = \chi_m + \chi_d$$

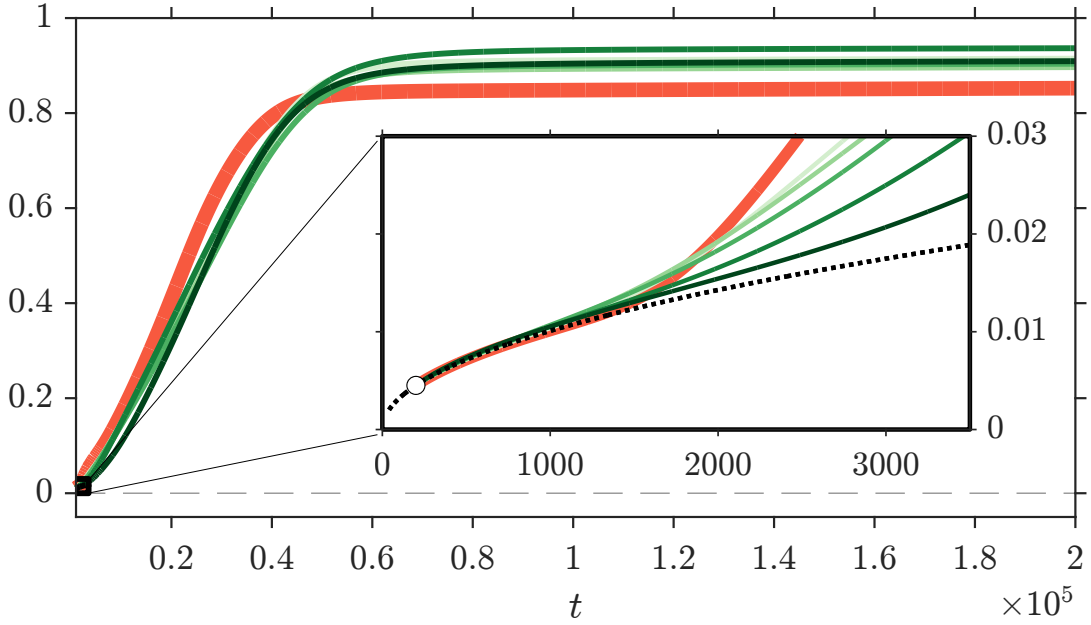


$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

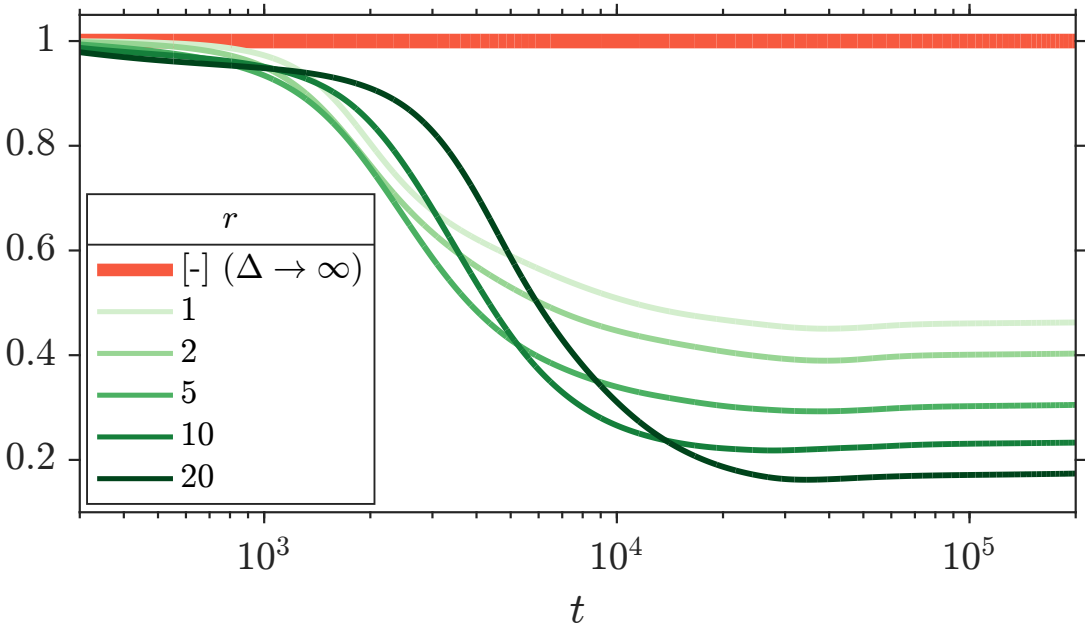
Degree of mixing

$$M_m(t) = \frac{2}{\sigma_{\max}^2 Ra} \int_0^t \chi_m \, \mathrm{d}\tau, \qquad M_d(t) = \frac{2}{\sigma_{\max}^2 Ra} \int_0^t \chi_d \, \mathrm{d}\tau$$

$M(t) = M_m(t) + M_d(t)$

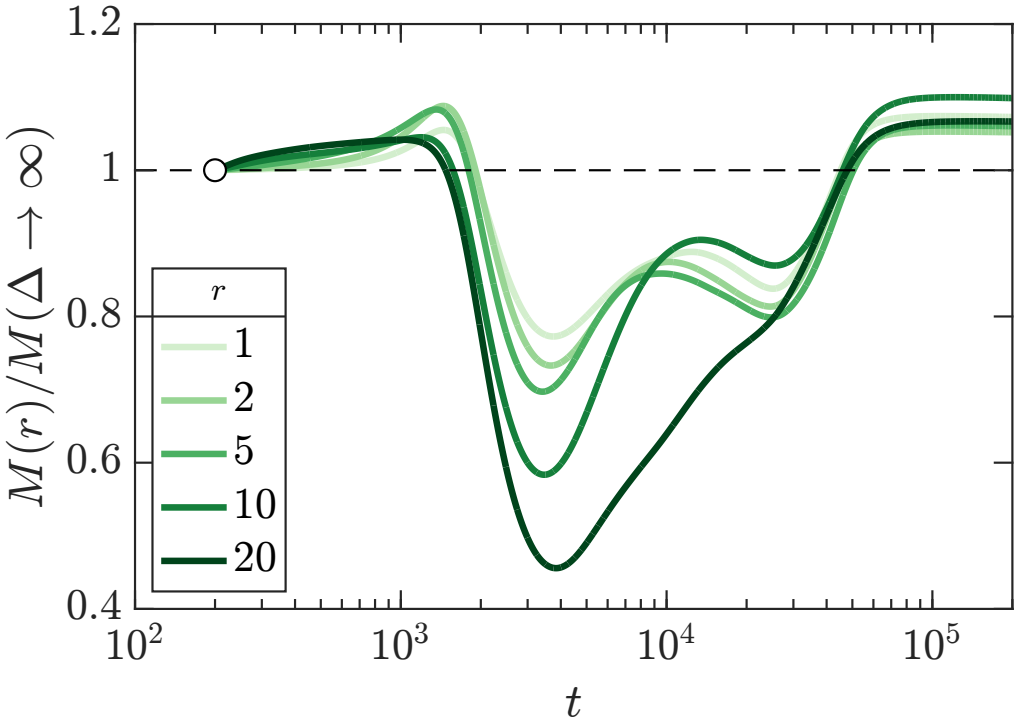


$M_m(t)\,/M(t)$

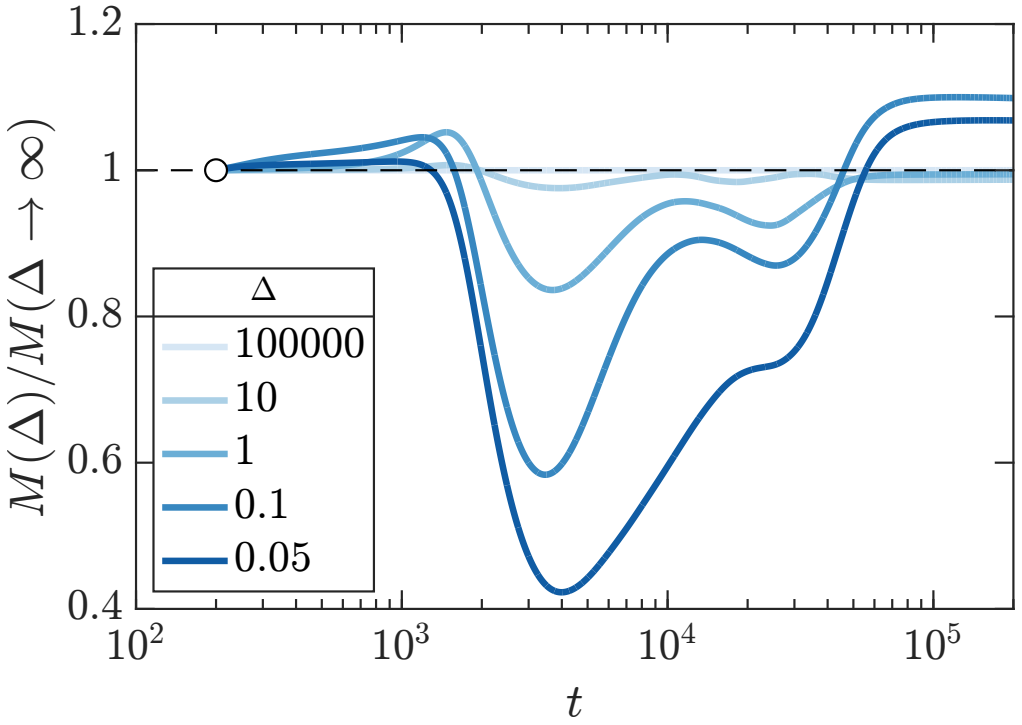


Degree of mixing

Effect of r ($\Delta = 0.1$)



Effect of Δ ($r = 10$)



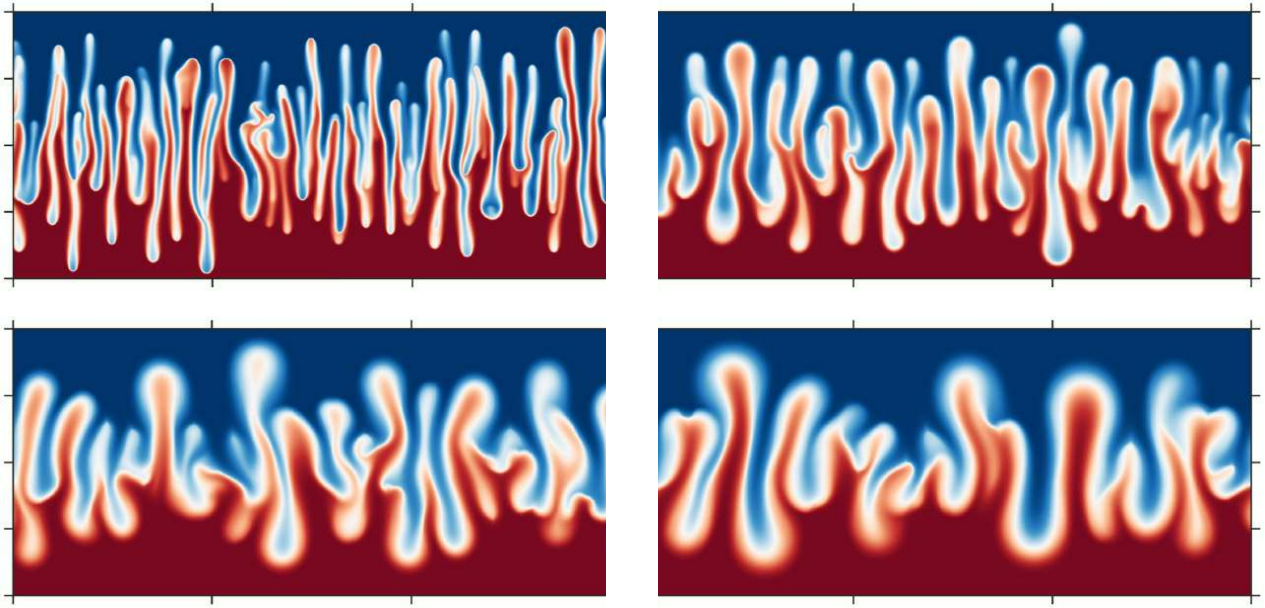
$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

Conclusions and outlook

Theoretical framework for convection in porous media with dispersion

Efficient open source code

Explain the behaviour of dispersion parameters, but parameters space is huge: need also to include experiments and new dispersion models



References

- De Paoli, M., Yerragolam, G. S., Verzicco, R. & Lohse, D. (*arxiv)* (2025).
- De Paoli, M., Yerragolam, G. S., Lohse, D. & Verzicco, R., *Computer Physics Communication* (2025).
- De Paoli, M., Howland, C. J., Verzicco, R., & Lohse, D., *Journal of Fluid Mechanics* (2024).

homepage and papers