# Multiscale modelling of convection in porous media:

## experiments, pore-scale and Darcy simulations with dispersion

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Physics of Fluids

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# Acknowledgements

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Physics of Fluids

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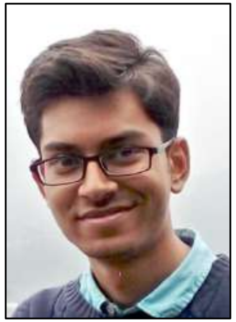

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This project has received funding from the European Union's Horizon Europe research and innovation programme under the Marie Sklodowska-Curie grant agreement MEDIA No. 101062123.

Funded by the European Union

European Commission

Marie Skłodowska-Curie Actions

MAX-PLANCK-GESELLSCHAFT

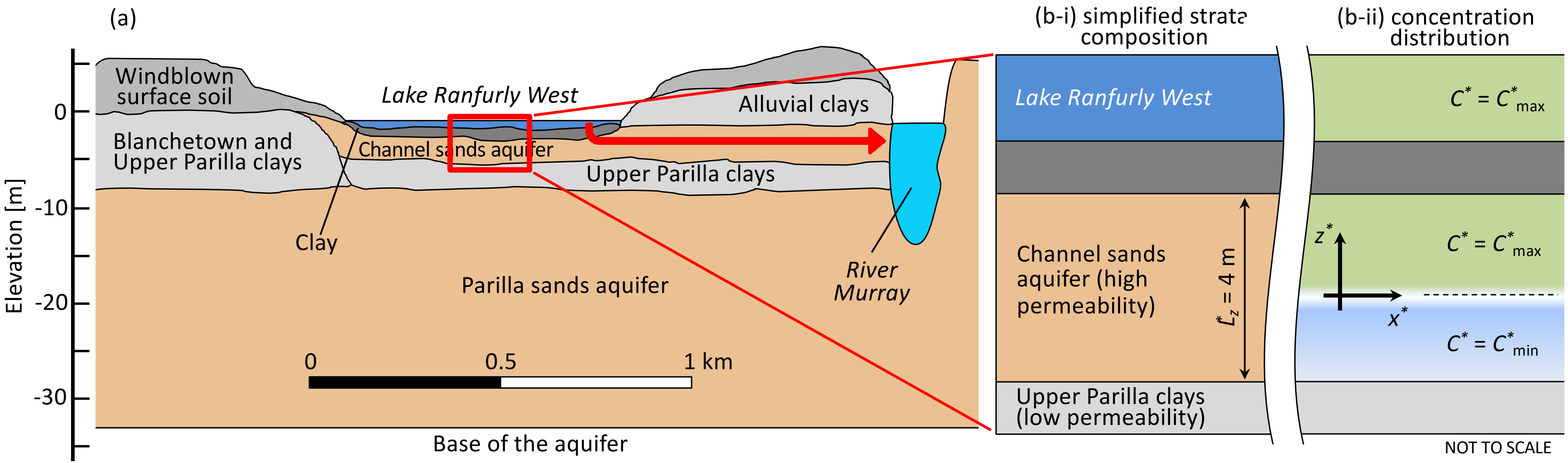
SURF

EuroHPC Joint Undertaking

# Motivation



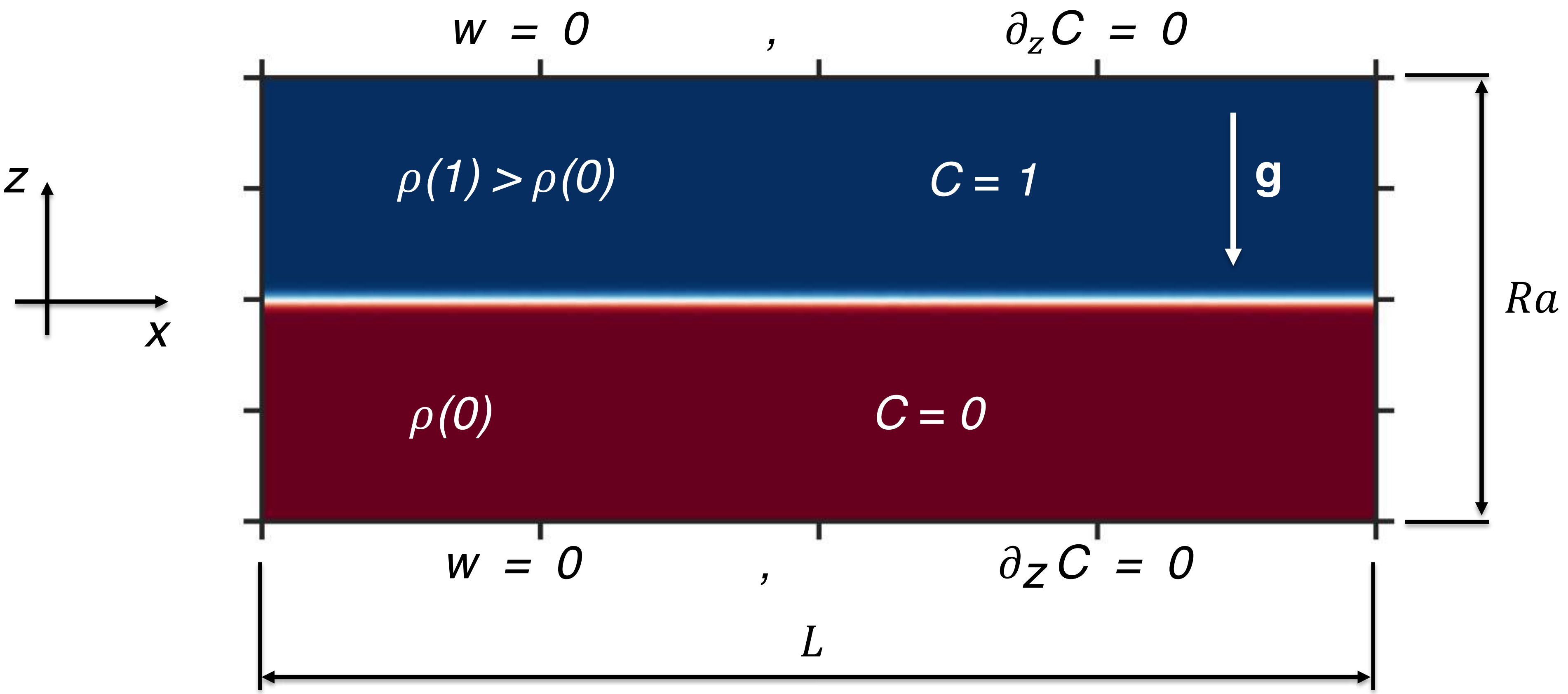
Conceptualized hydrogeology of the River Murray basin area, adapted from Narayan, K.A. & Armstrong, D., *J. Hydrol.* 165 (1-4), 161–184.




In case of low streams, high salinity in the river makes the water unusable for agriculture ⇒ Crucial to predict dispersion effects and effectively design and manage water resources

# Flow configuration





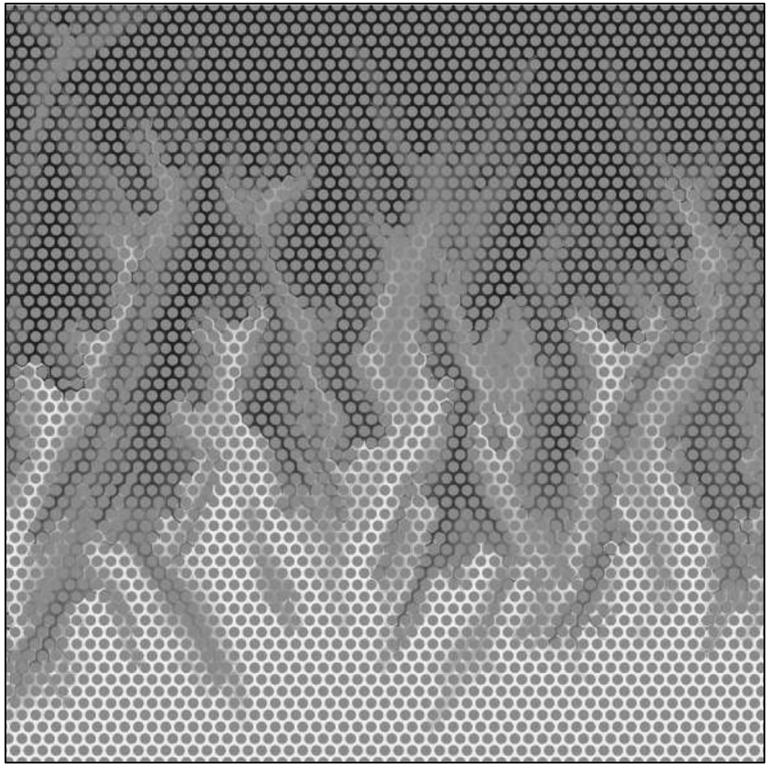
# Simulations



## pore-scale

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

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



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

# Simulations

pore-scale

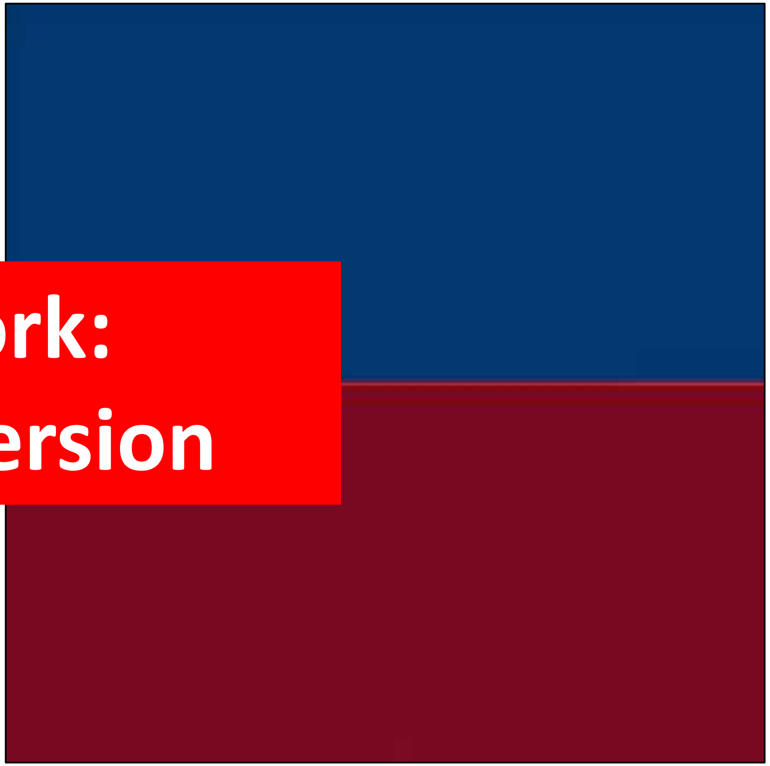
$$\partial_t \boldsymbol{u} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = -\rho_0^{-1} \nabla p + \nu \nabla^2 \boldsymbol{u} - g\beta C \hat{\boldsymbol{z}},$$

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

Darcy scale

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

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



**Aim of this work: Buoyancy + Dispersion**

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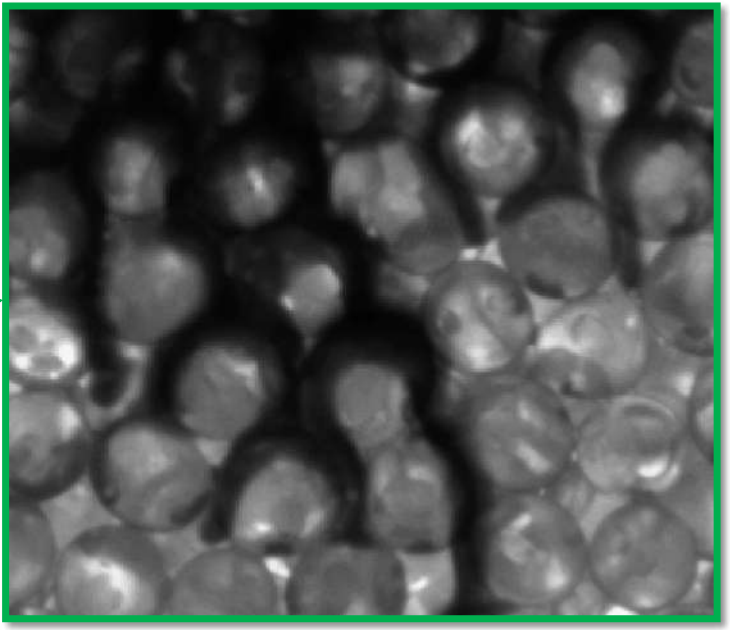
# Governing equations

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

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

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



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

**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**

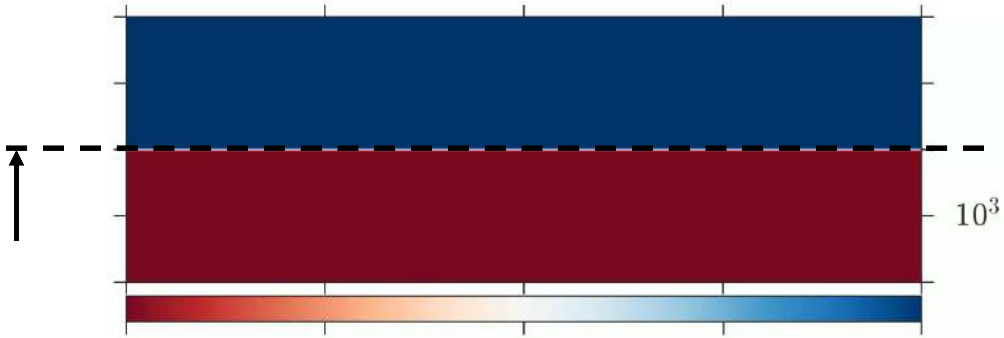
$$\Delta = \frac{D_m^*}{D_t^*} \quad , \quad r = \frac{D_l^*}{D_t^*} = \frac{\alpha_l^*}{\alpha_t^*}$$

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

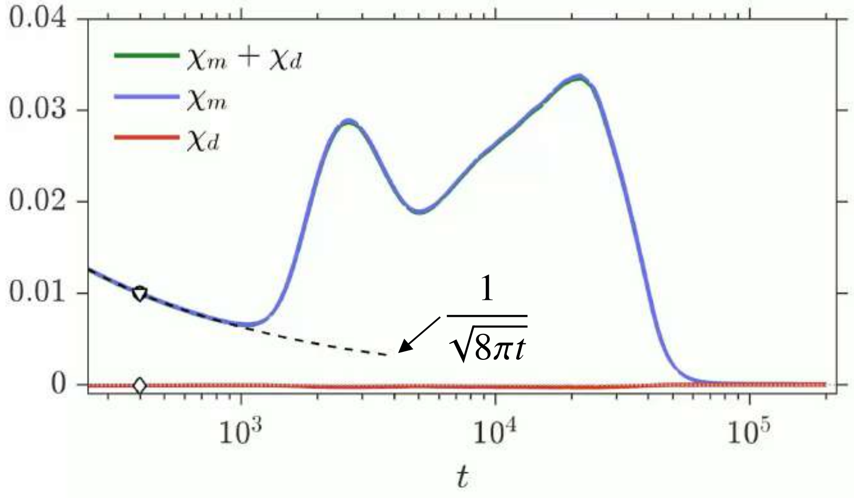
# No dispersion ($\Delta \to \infty$)

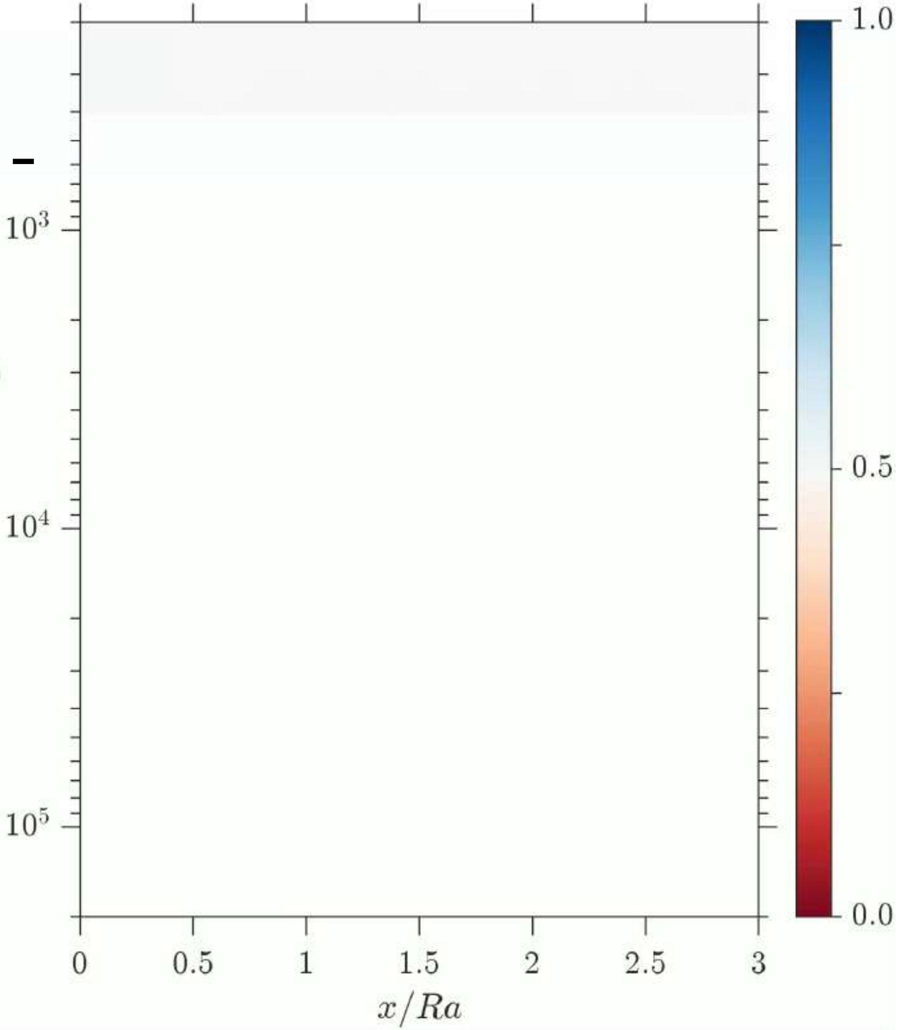
$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^T}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$



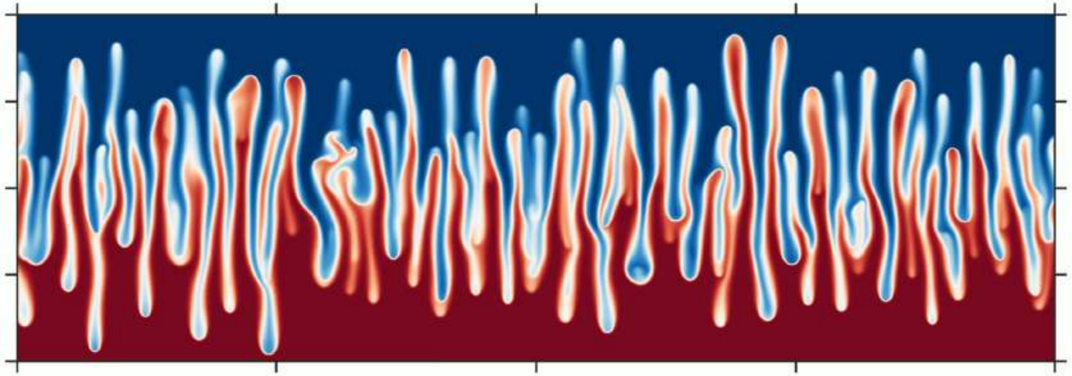



$$\chi_m = Ra\langle|\nabla C|^2\rangle, \quad \chi_d = Ra\langle(\nabla C)\cdot(\boldsymbol{D}\nabla C) - |\nabla C|^2\rangle$$

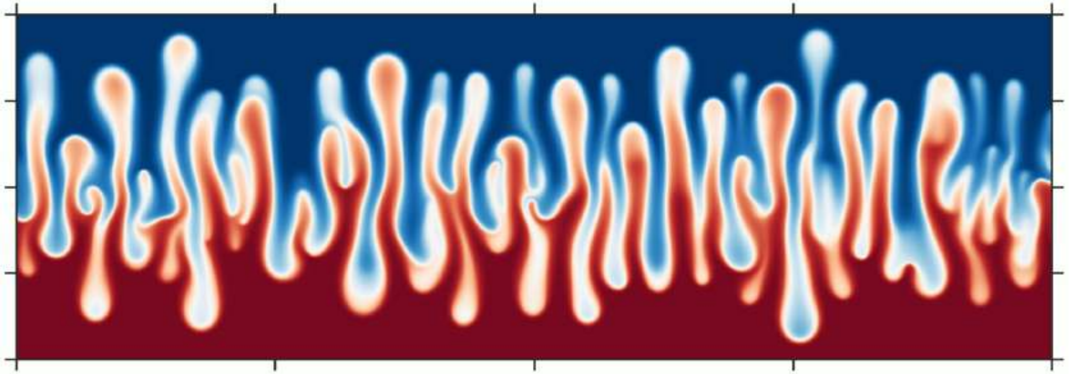


# variable $r, \Delta = 0.1, \mathrm{Ra} = 10^4$



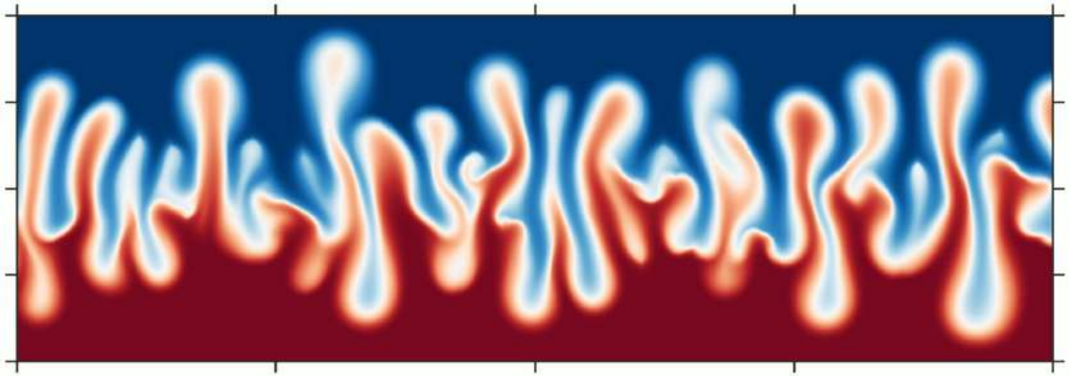
No dispersion



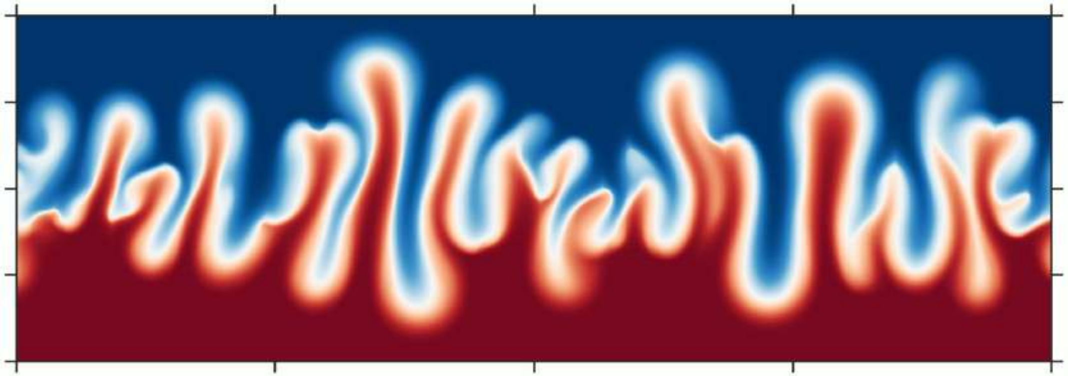
$r = 1$

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

$r = 10$



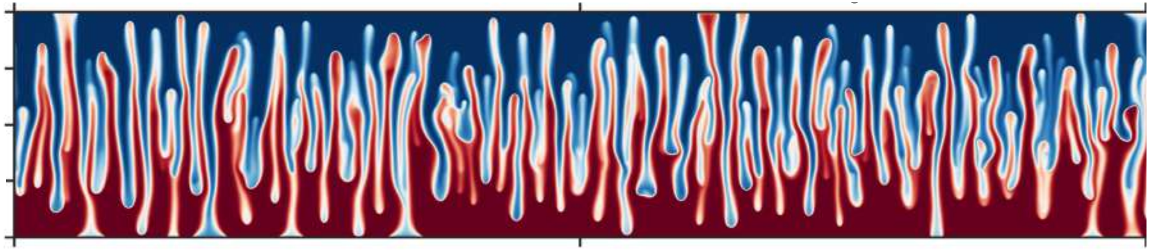
$r = 20$



# Molecular dissipation

(a)

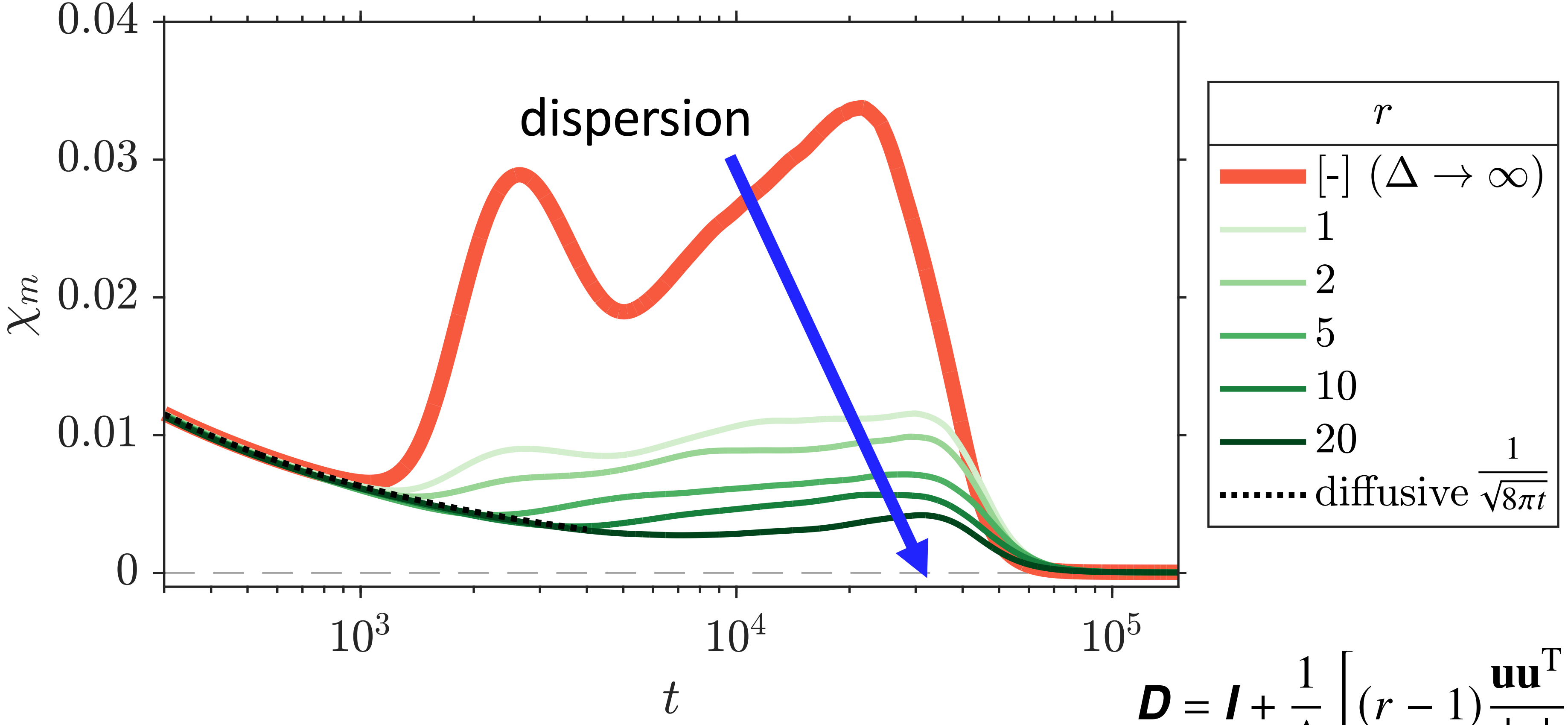
No dispersion



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

Gradient across the interface of the fingers reduces

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

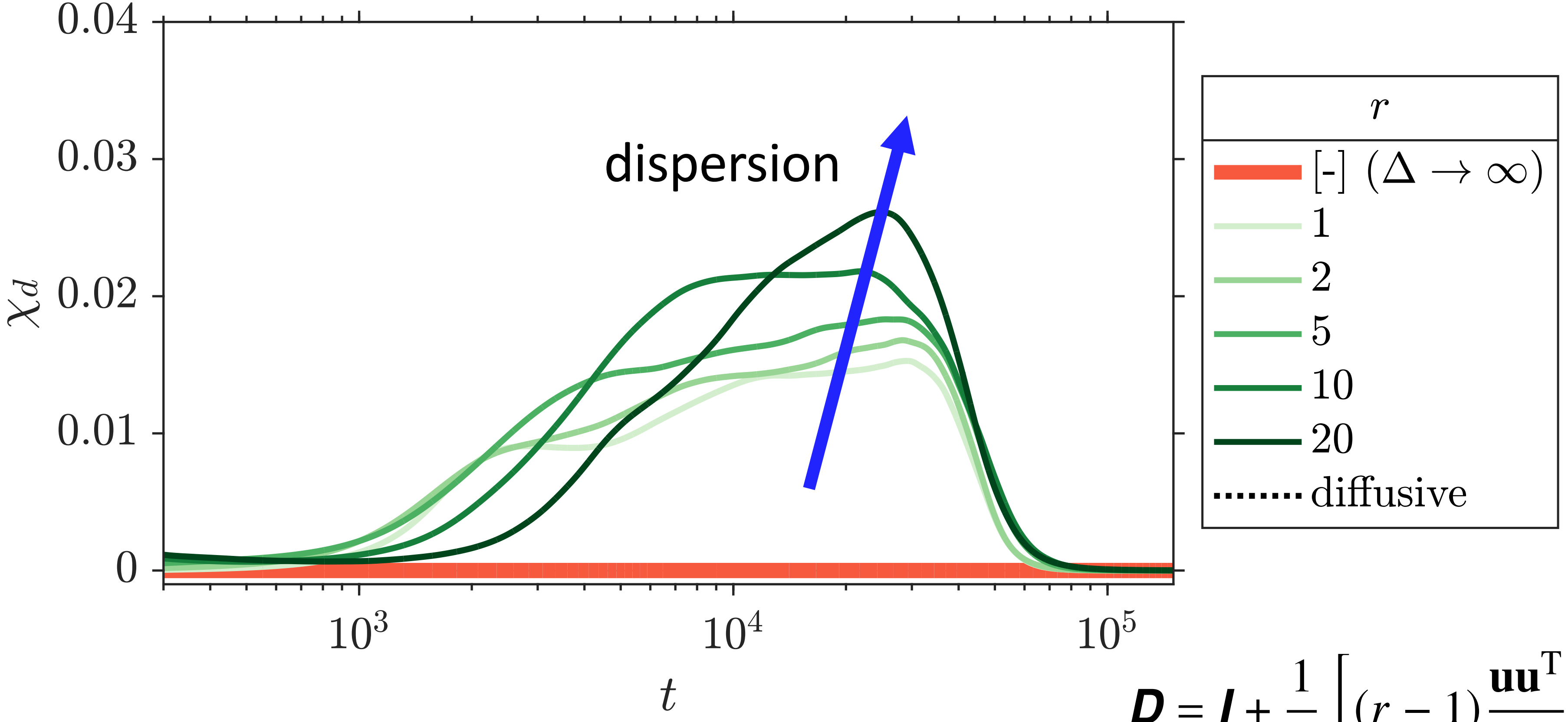



$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

# Dispersive dissipation



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

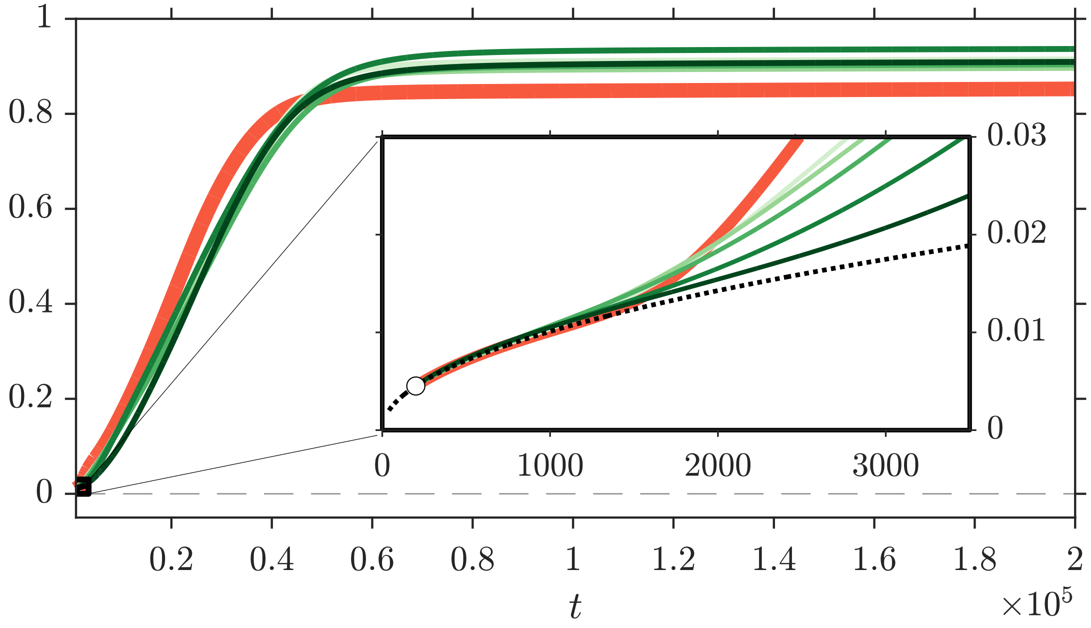



$$\boldsymbol{D} = \boldsymbol{I} + \frac{1}{\Delta}\left[(r-1)\frac{\mathbf{u}\mathbf{u}^{\mathrm{T}}}{|\mathbf{u}|} + \boldsymbol{I}|\mathbf{u}|\right]$$

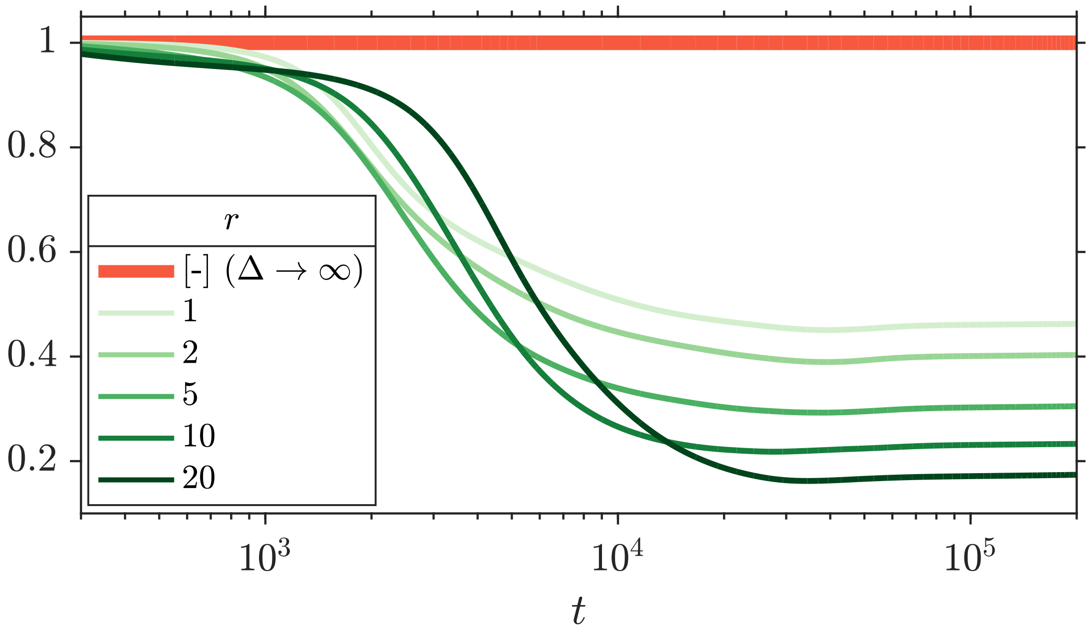
# Degree of mixing

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

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

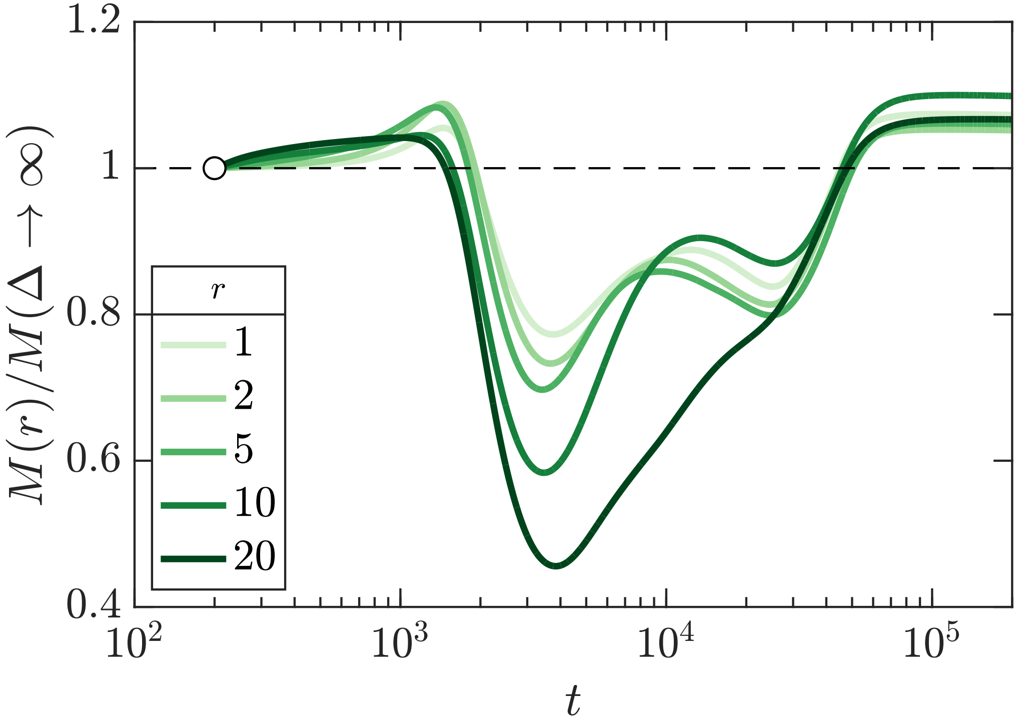



$M_m(t)/M(t)$

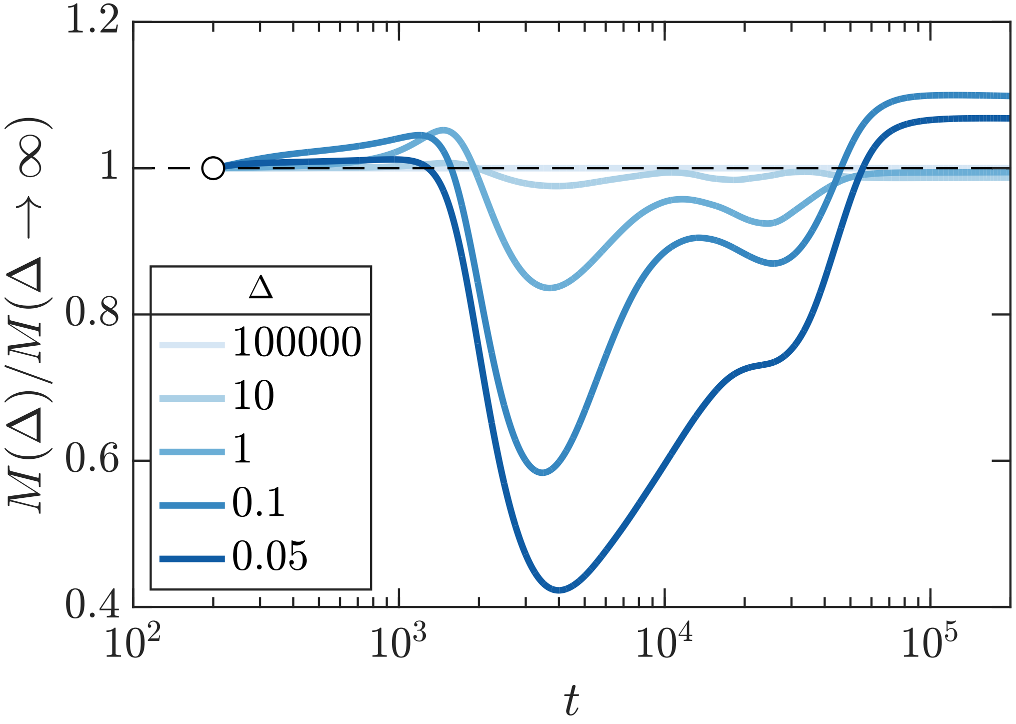


# Degree of mixing

## Effect of *r* (Δ = 0.1)

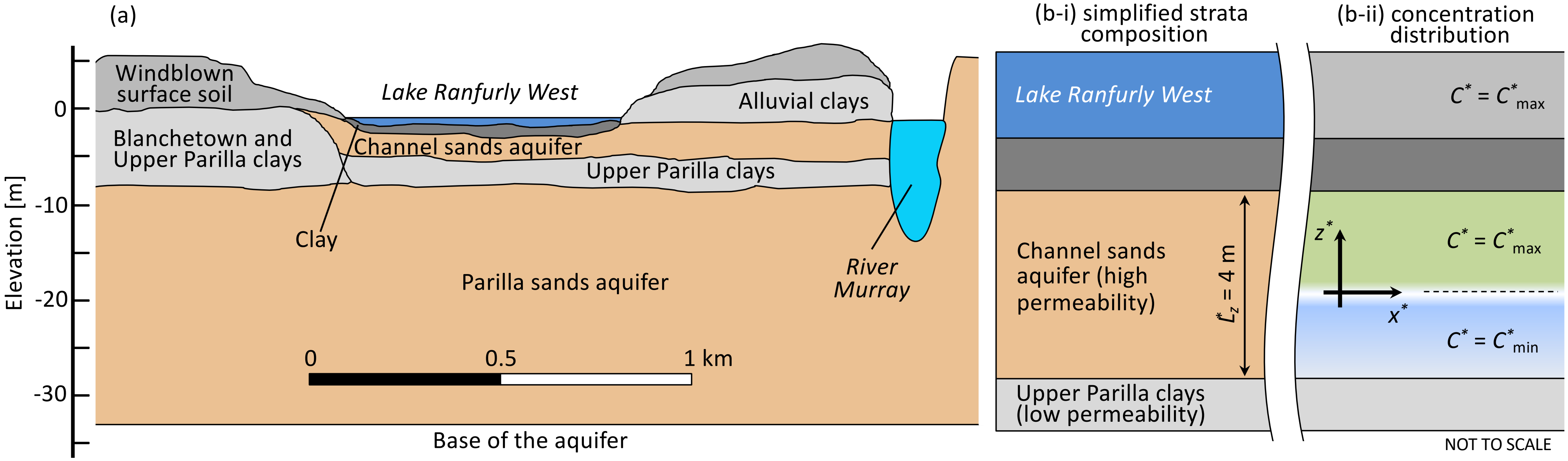



## Effect of Δ (*r* = 10)




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

# Motivation




**fluid properties**

$$\mu = 10^{-3} \text{ Pa s}$$
$$\Delta\rho^* = 52.5 \text{ kg/m}^3$$

**medium properties**

$$k = 2.95 \times 10^{-11} \text{ m}^2$$
$$\phi = 0.3$$
$$\alpha_l^* = 80 \text{ m}$$
$$L_z^* = 4 \text{ m}$$

**dimensionless parameters**

$$r = 10$$
$$\Delta = r D_m / (\mathscr{U}^* \alpha_l^*) \approx 10^{-5}$$
$$Ra = 1.35 \times 10^5$$

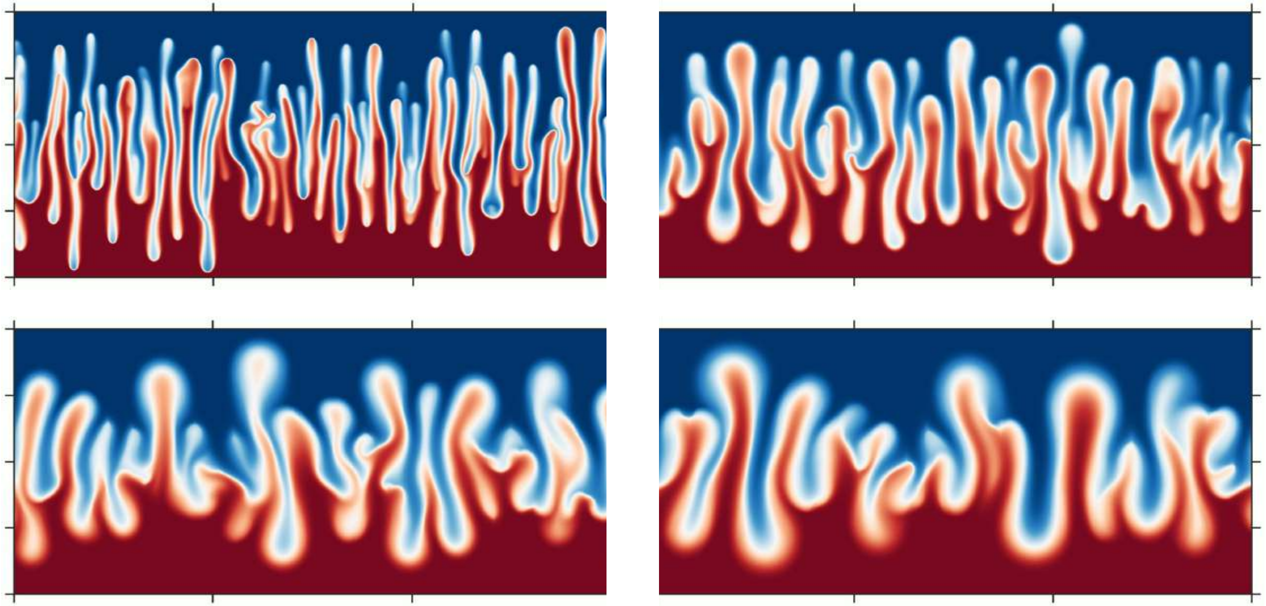
Dispersion dominates and it has to be taken into account

$$\mathscr{U}^* = 1.52 \times 10^{-5} \text{ m/s} = 1.31 \text{ m/d}$$

# 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).

**preprint**

High-resolution images, movies and slides are available upon request to marco.de.paoli@tuwien.ac.at