PoreLab
NTNU-UiO Porous Media Laboratory

Norwegian Centre of Excellence
The Research Council of Norway

NTNU

UiO : University of Oslo

Onsager symmetries in miscible fluid flow

Eirik G. Flekkøy, Steve Pride and Renaud Toussaint

Ongoing studies on dispersion

Onsager: Connecting the micro and the macro on the basis of time-reversibility at the meso-level

Point source-receiver symmetry and dispersive focusing and prediction

Hydrodynamic dispersion and coarse graining – the upscaling problem

Symmetries of the dispersion tensor

Possible macroscopic dispersion tensors

22.08.2019

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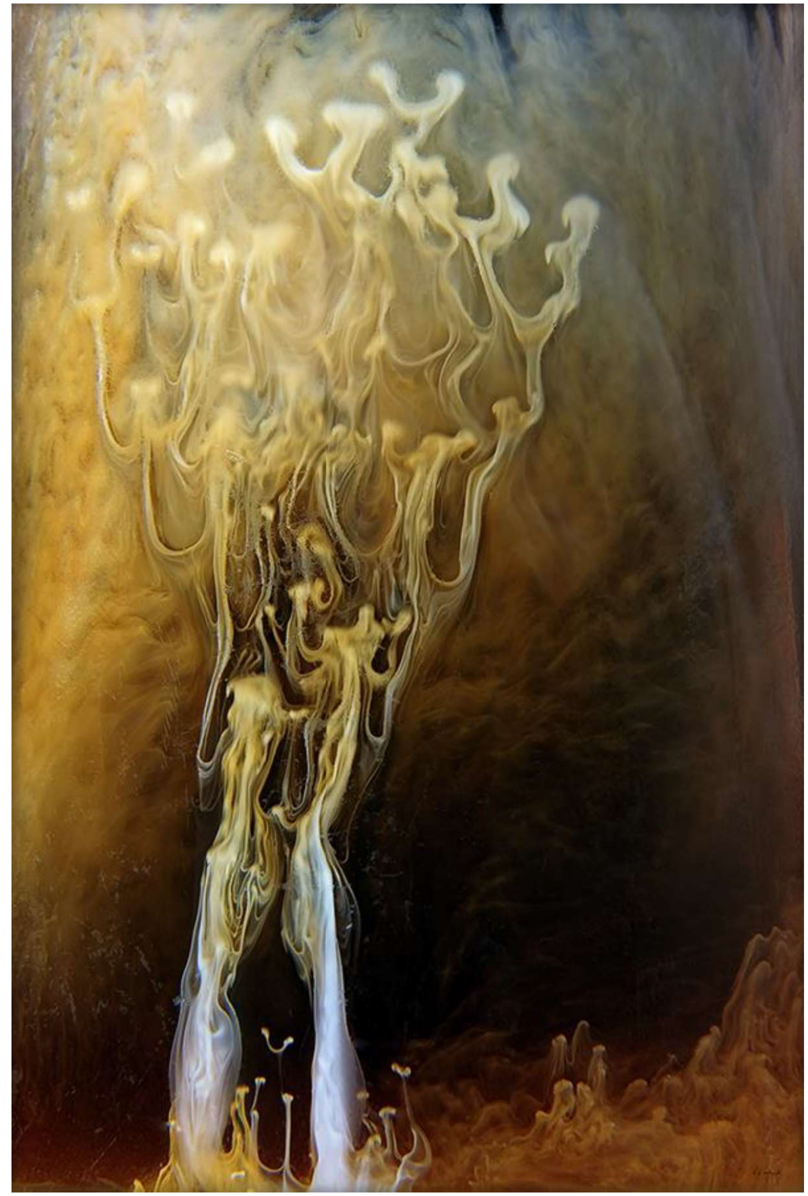
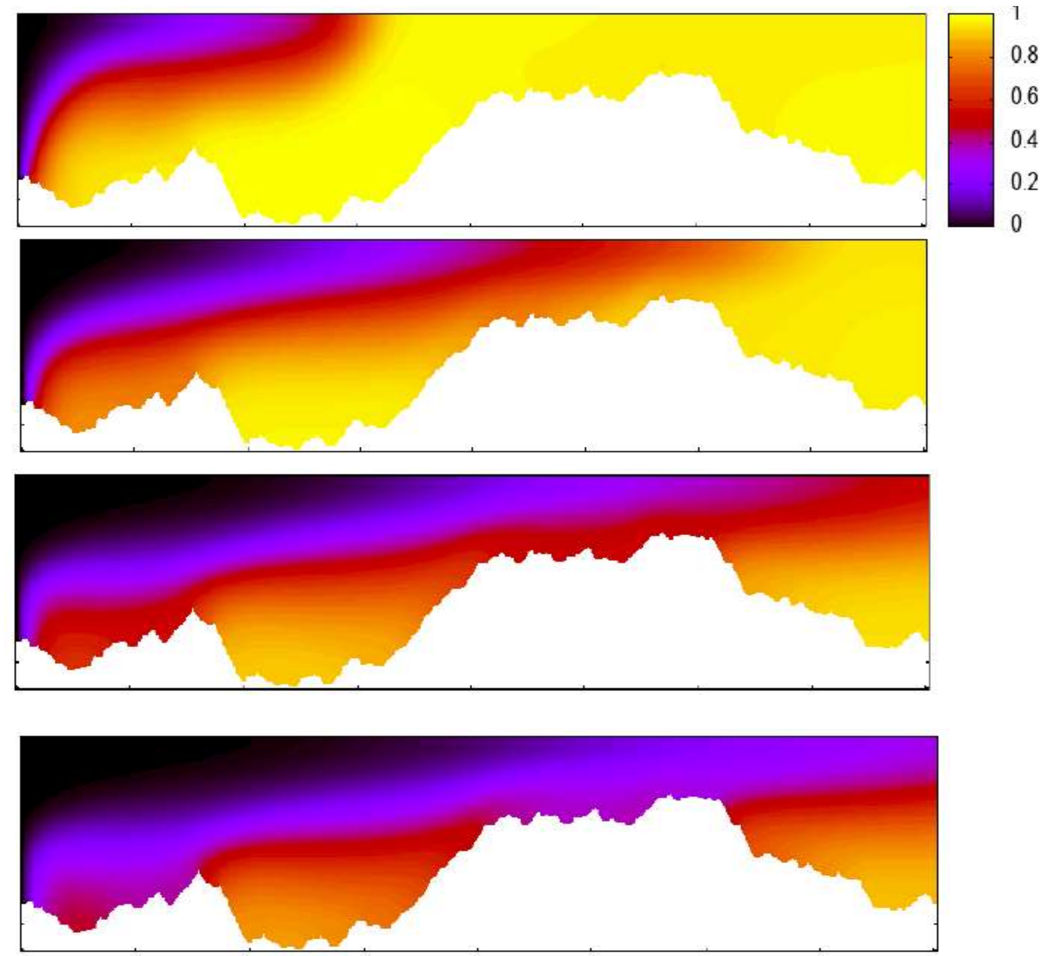
Hydrodynamic dispersion

- Whenever advection with a flow and molecular diffusion combines



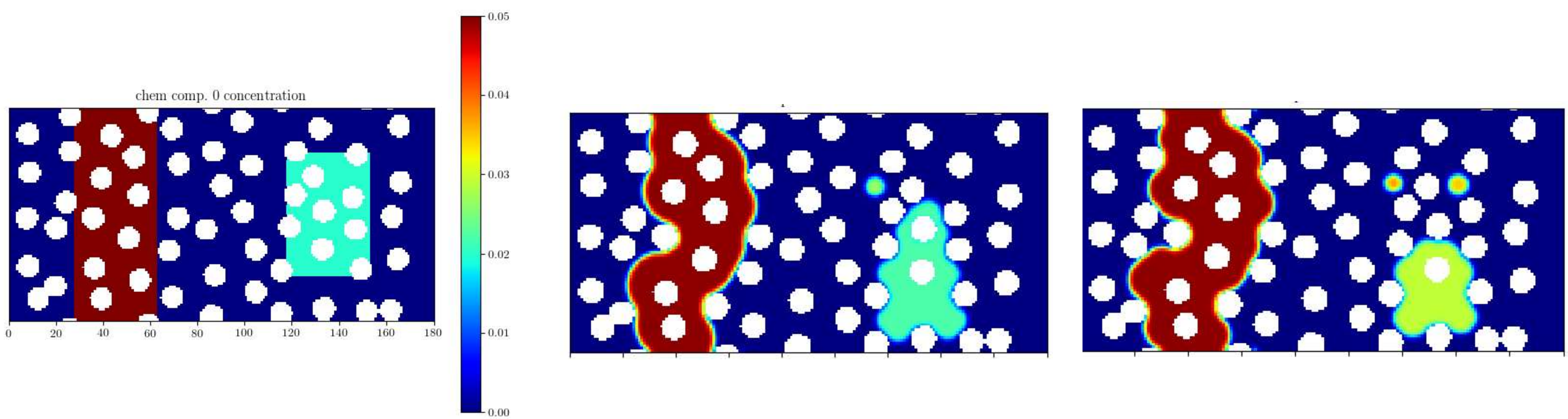
Thermally stabilized flow over rough surfaces

- Beatrice Baldelli (UiO)

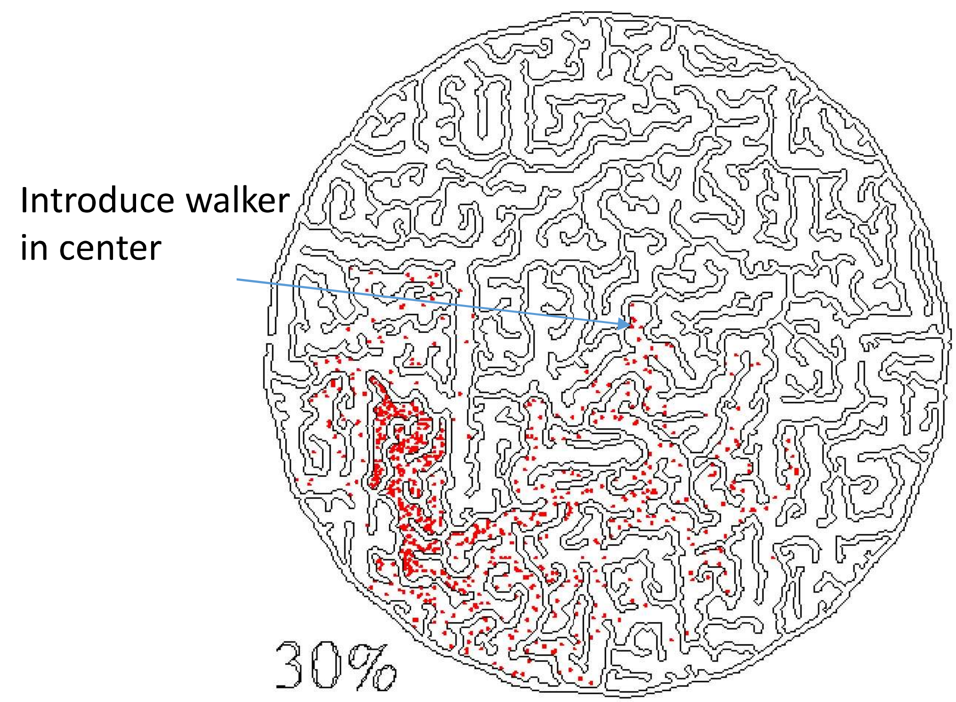


Flow in porous media driven by osmotic effects and associated Lattice Boltzmann models for partially miscible fluids

- Carl Fredrik Berg (NTNU), Mohammed Hossein Golestan (NTNU), Olav Aursjø (IRIS) and Ole Thorseter (NTNU)

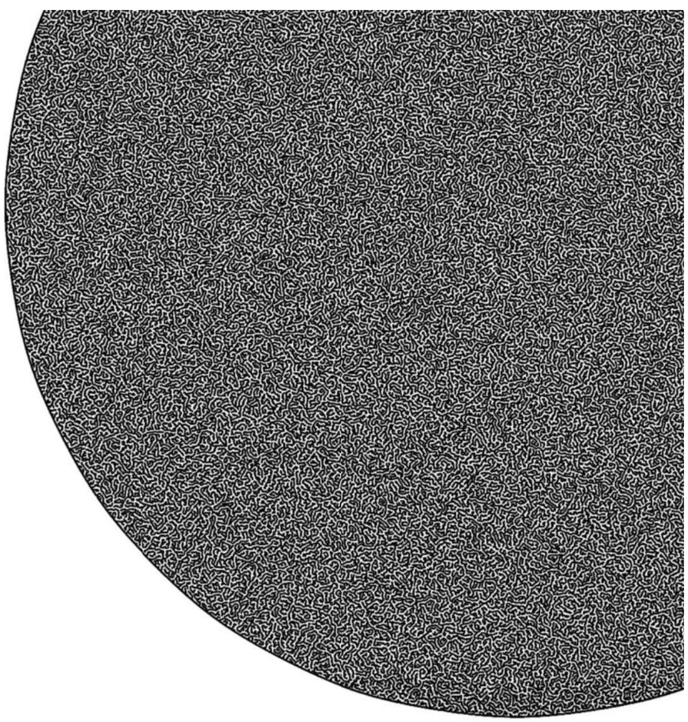


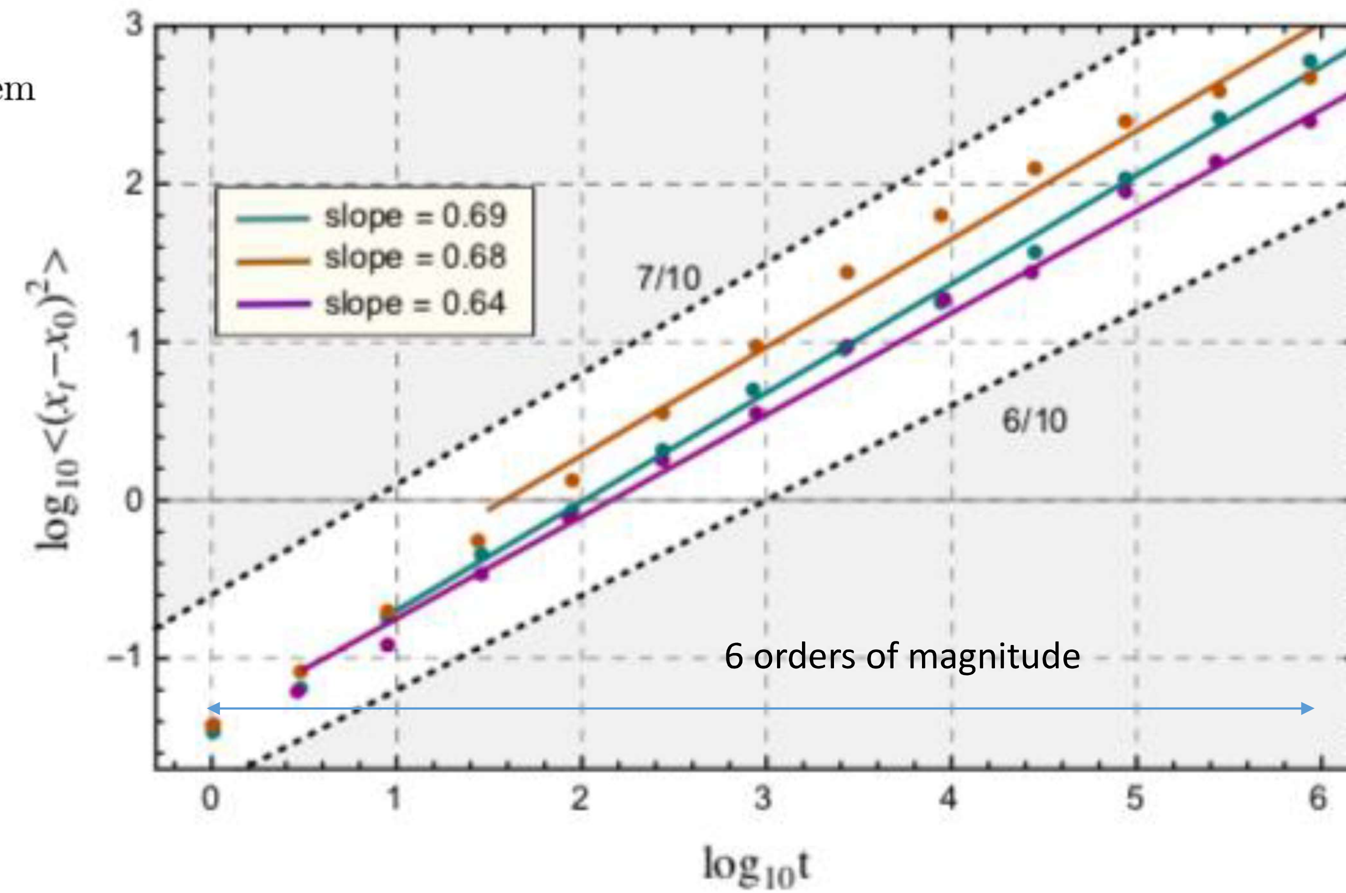
Random walk on labyrinth



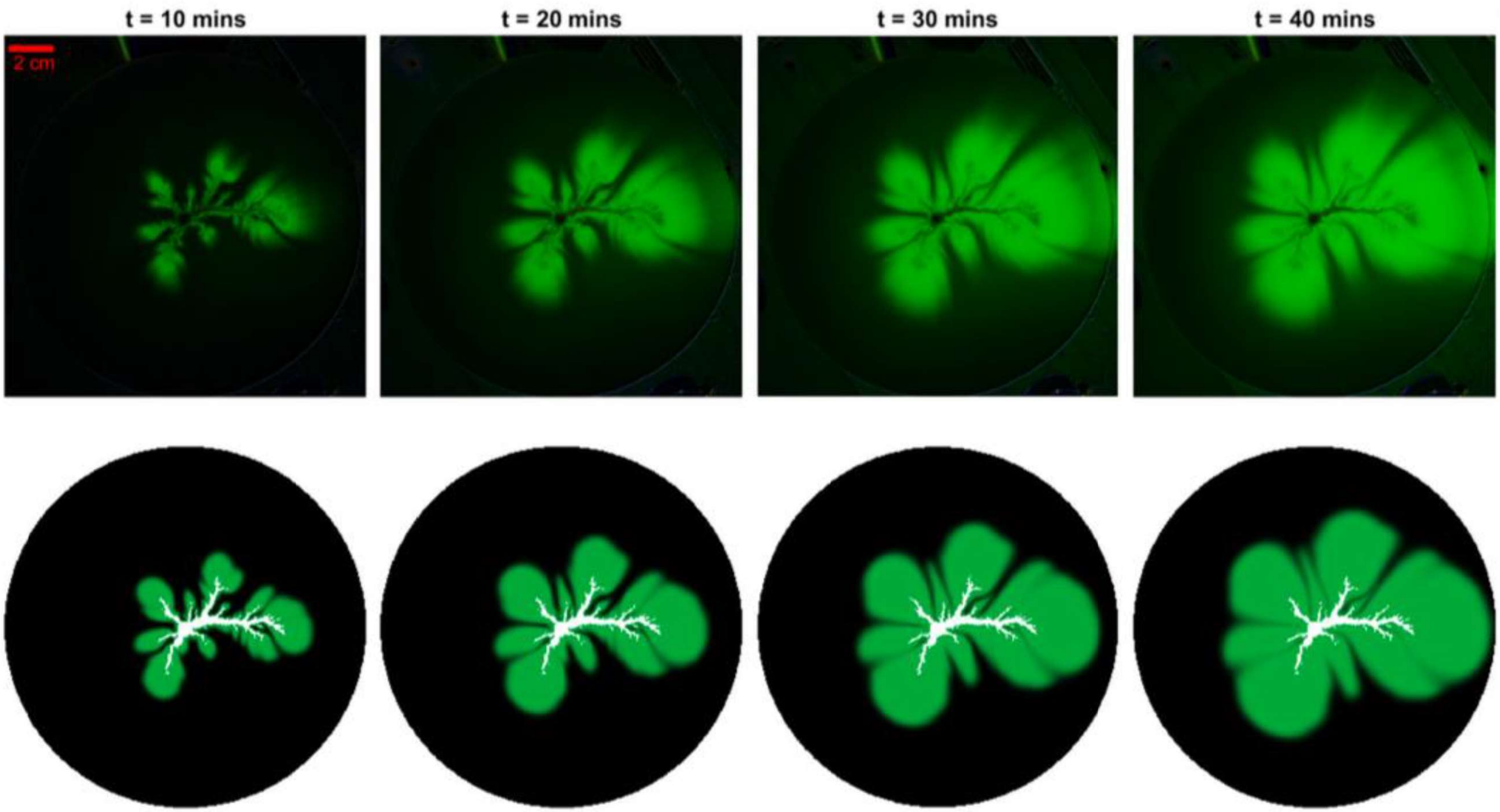
Anomalous diffusion $\langle r^2(t) \rangle \sim t^{\alpha}$

$\alpha = 0.69,\ 0.68, \ldots 0.64$ for the largest system





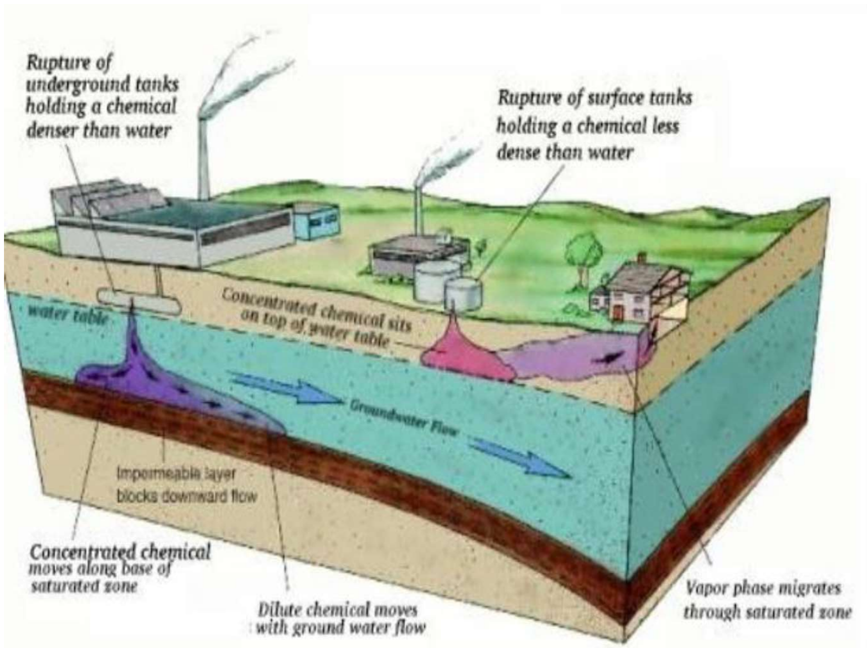
Flow from a dissolution pattern

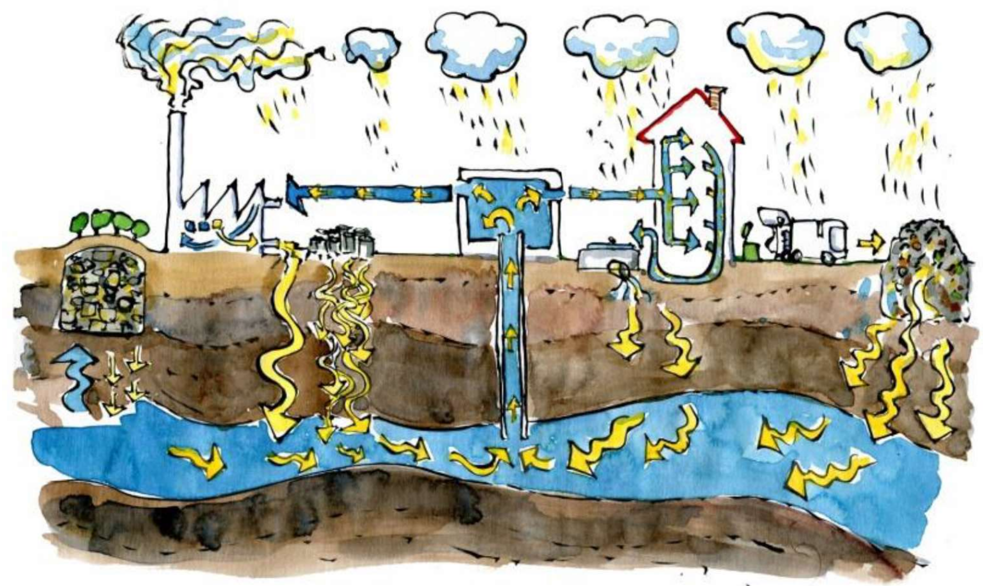


Le Xu and Knut Jørgen Måløy

Hydrodynamic dispersion

- Ground water pollution





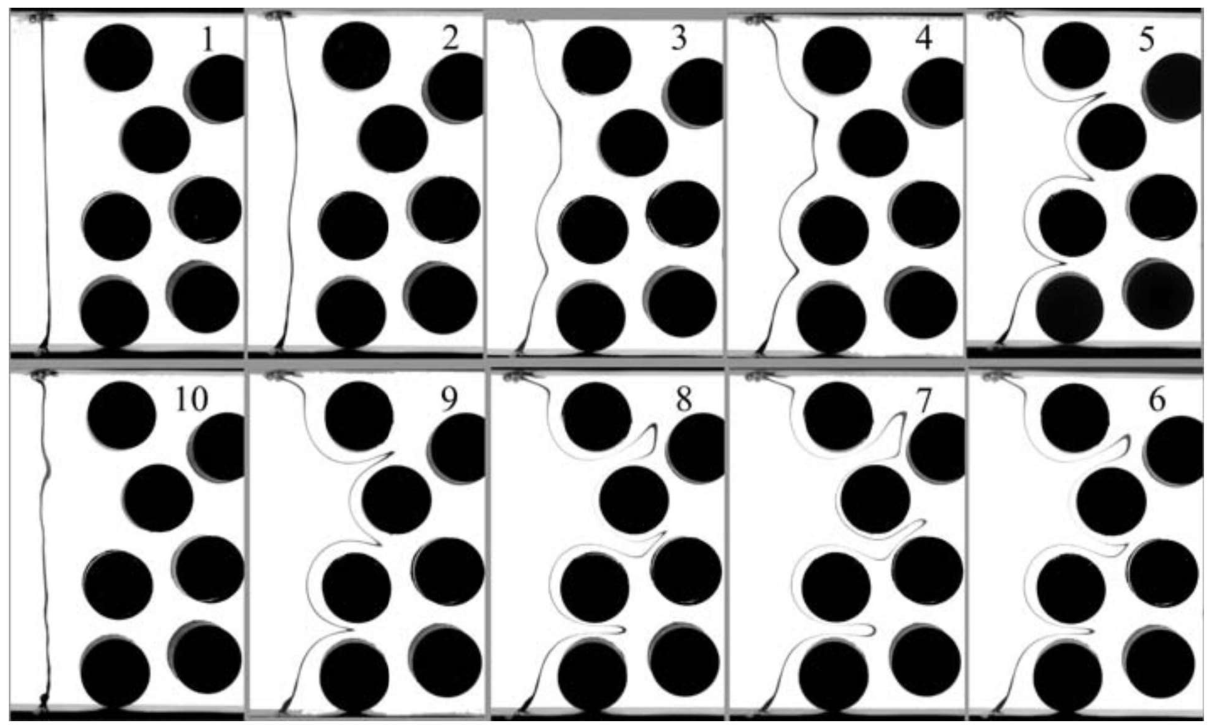
Hydrodynamic dispersion

- In biological systems

Gunther von Hagens *Bodyworld*

Hydrodynamic dispersion

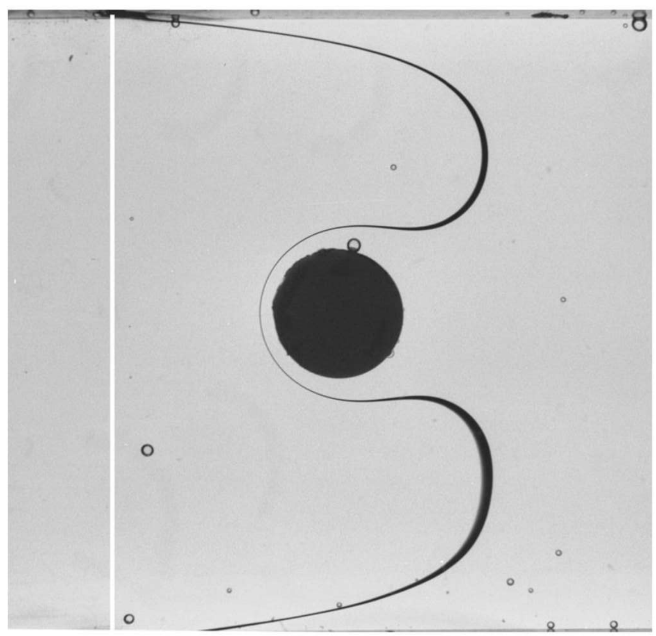
- Reversible dispersion if molecular diffusion is sufficiently weak

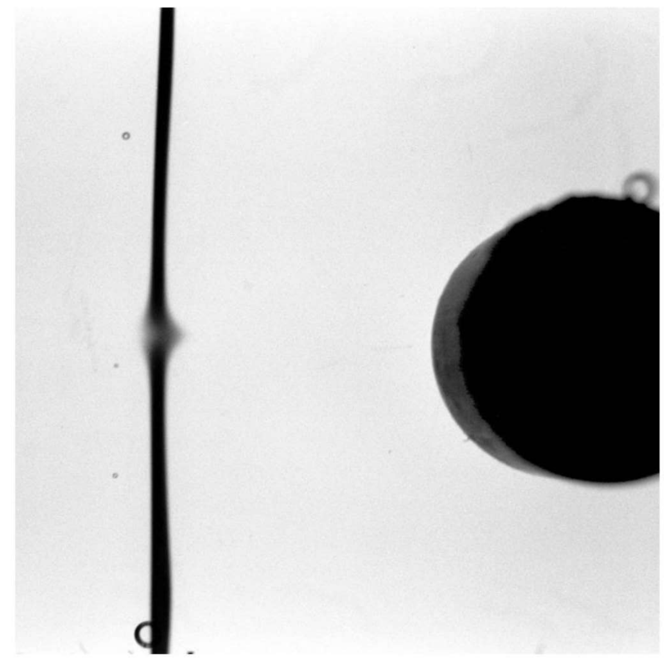


Jens Feder

Hydrodynamic dispersion

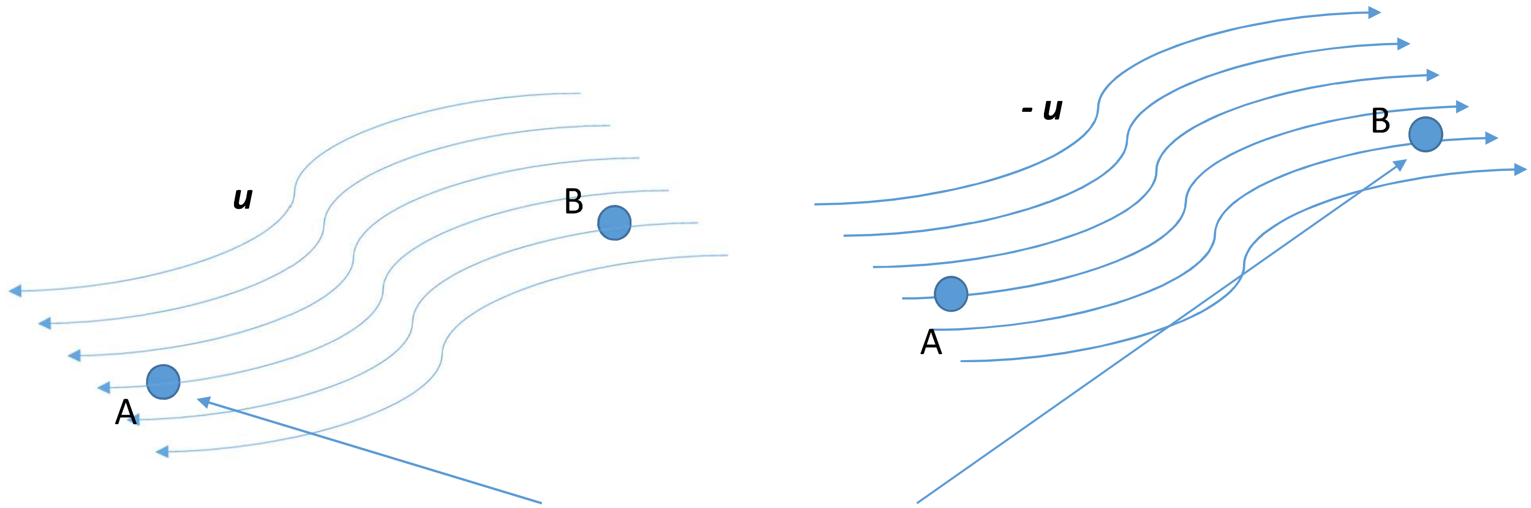
- Reversible dispersion if molecular diffusion is sufficiently weak





Oxaal, Flekkøy, Feder PRL 1993

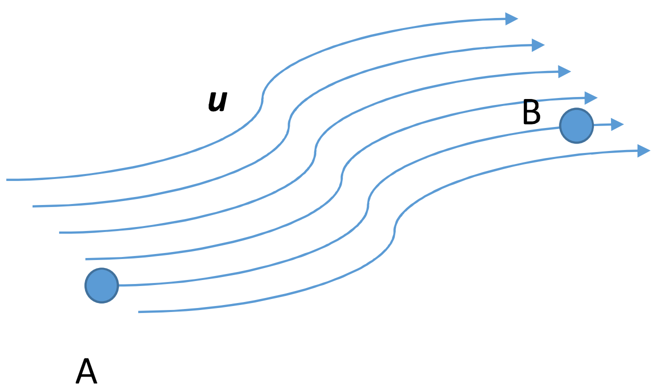
Reversibility on the pore-level: Source and receiver symmetry under flow reversal



$$\frac{C_B(\mathbf{x}_A, t)}{m_{B0}} = \frac{C_A(\mathbf{x}_B, t)}{m_{A0}}$$

E.G. Flekkøy Phys. Fluids **9** 1997

Reciprocity may be shown directly from the diffusion equation



$$\frac{\partial C_A}{\partial t} = -\nabla \cdot \mathbf{j}_A + m_0 \delta(t)\, \delta(\mathbf{x} - \mathbf{x}_A)$$

$$\mathbf{j}_A = -D \nabla C_A + \mathbf{u} \; C_A$$

.. .but we will instead follow an ‘Onsager route’:

Time reversible microdynamics implies:

Time reversal invariance in this case means that if a motion picture showing all the particles moving according to the background field $\mathbf{u}(\mathbf{x})$, were shown backwards, it could not by means of statistical analysis be distinguished from a film with a background field $-\mathbf{u}(\mathbf{x})$, which was shown in the forward direction.

Time reversibility means that the correlation function is even in *t, so:*

$$\langle \Delta\tilde{m}(\mathbf{x}_B, t)\Delta\tilde{m}(\mathbf{x}_A, 0)\rangle = \langle \Delta\tilde{m}^-(\mathbf{x}_A, t)\Delta\tilde{m}^-(\mathbf{x}_B, 0)\rangle,$$

Split average in one over mass at A, then over different responses to that mass:

$$\langle \Delta\tilde{m}(\mathbf{x}_B, t)\Delta\tilde{m}(\mathbf{x}_A, 0)\rangle = \sum_{\tilde{m}(\mathbf{x},0)} P[\tilde{m}(\mathbf{x},0)]\langle \Delta\tilde{m}(\mathbf{x}_B, t)\Delta\tilde{m}(\mathbf{x}_A, 0)\rangle_{\tilde{m}(\mathbf{x},0)}$$

$$\langle \Delta\tilde{m}(\mathbf{x}_B, t)\Delta\tilde{m}(\mathbf{x}_A, 0)\rangle = \langle \Delta\tilde{m}^2(\mathbf{x}_A, 0)\rangle R(\mathbf{x}_B, \mathbf{x}_A, t)\Delta v$$

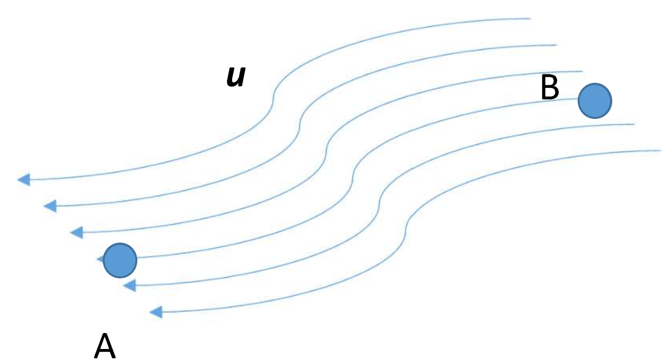
↑

$$R = C_A(\mathbf{x}_B, t)/m_0$$

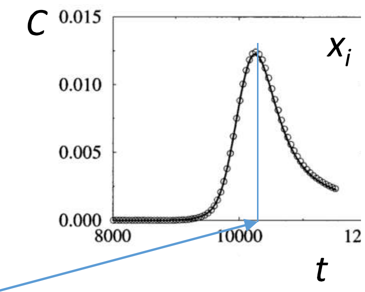
Time reversibility leads to reciprocity

$$\langle \Delta \widetilde{m}(\mathbf{x}_B, t)\Delta \widetilde{m}(\mathbf{x}_A, 0)\rangle = \langle \Delta \widetilde{m}^-(\mathbf{x}_A, t)\Delta \widetilde{m}^-(\mathbf{x}_B, 0)\rangle,$$

$$\frac{C_B(\mathbf{x}_A, t)}{m_{B0}} = \frac{C_A(\mathbf{x}_B, t)}{m_{A0}}$$



An echo simulation maximizing $C(x_A, T)$



Injected mass $m(\mathbf{x}_i) = aC(\mathbf{x}_i, t_M(\mathbf{x}_i))$ at a time according to the

first-in-last-out rule $t_I(\mathbf{x}_i) = T - t_M(\mathbf{x}_i)$

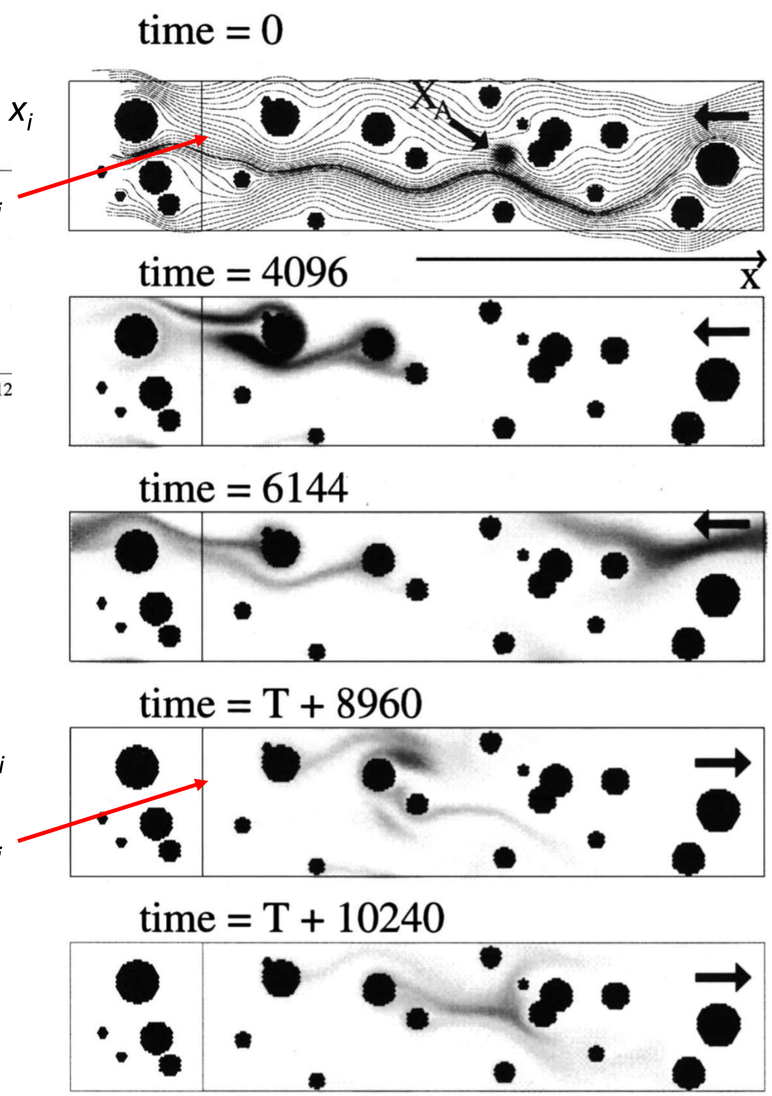
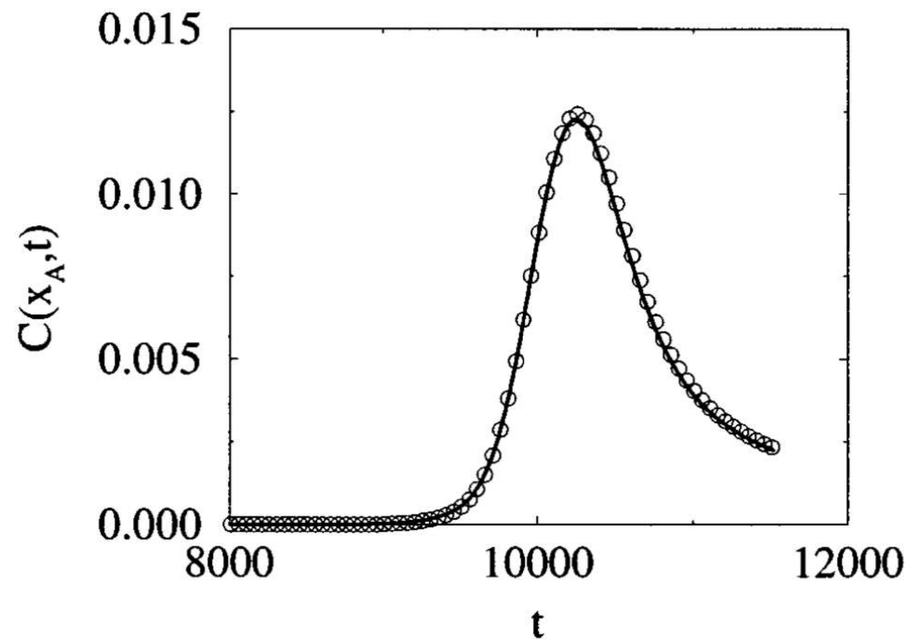


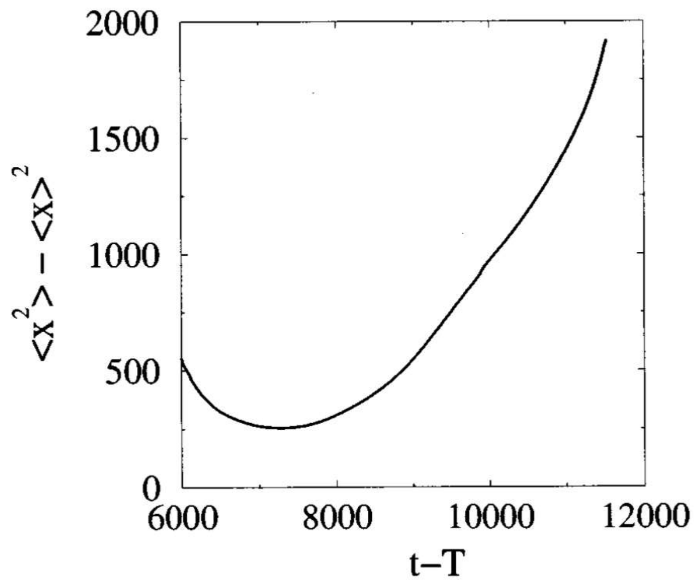
FIG. 1. The tracer concentration resulting from a point source at $\mathbf{x}_A$ (first 3

Predicted concentration:

$$C_{\rm th}(\mathbf{x}_A, t) = \sum_i R(\mathbf{x}_i, \mathbf{x}_A, t - t_I(\mathbf{x}_i))\, m(\mathbf{x}_i)$$



Focusing effect



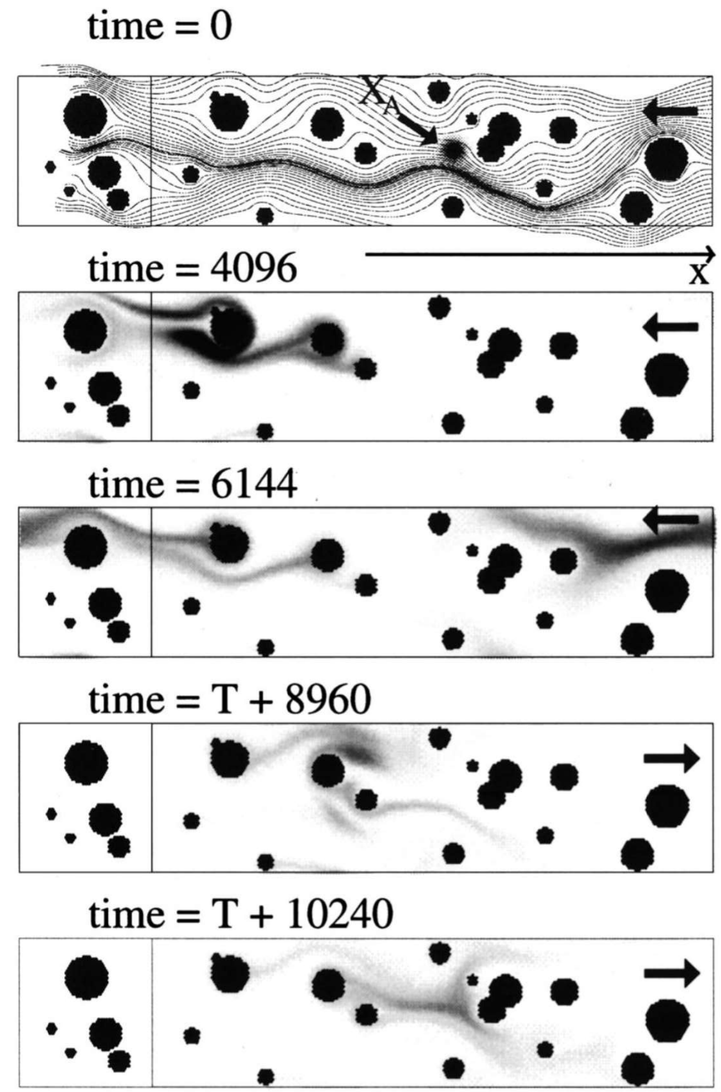
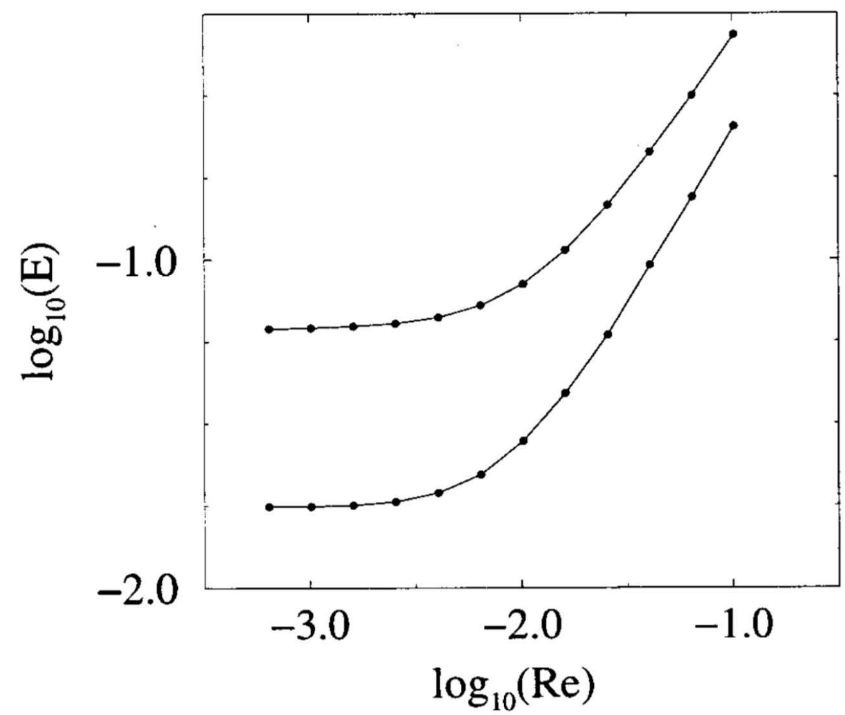


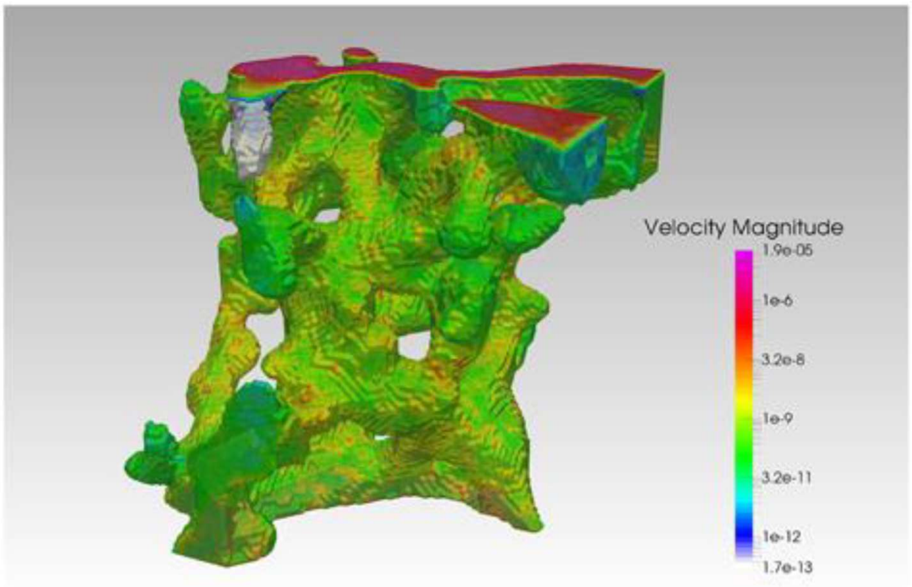
FIG. 1. The tracer concentration resulting from a point source at $\mathbf{x}_A$ (first 3

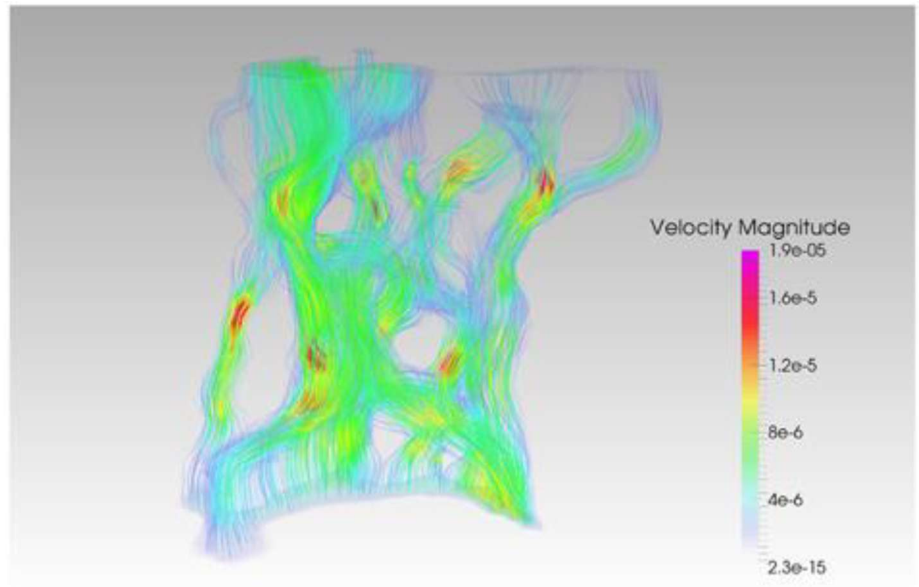
Deviation E from prediction at finite Re



Coarse graining hydrodynamic dispersion

- Generally, the dispersion tensor characterizes the porous medium and the fluids in it

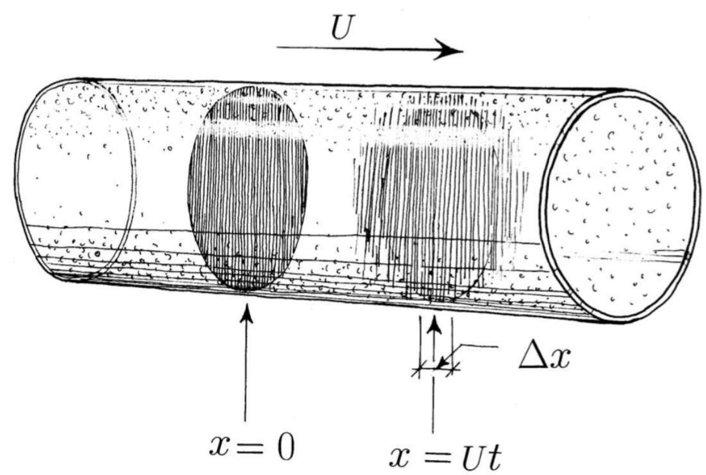




M. Misztal et al

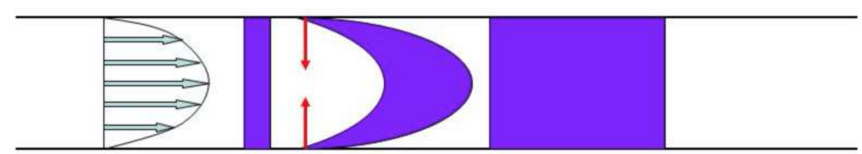
Hydrodynamic dispersion

- Taylor dispersion



$$\mathbf{J} = \rho_0 \overline{\mathbf{U}} - \mathbf{D} \cdot \boldsymbol{\nabla} \rho_0,$$

$$D_{\|} = \frac{a^2 U^2}{48 D_m}$$

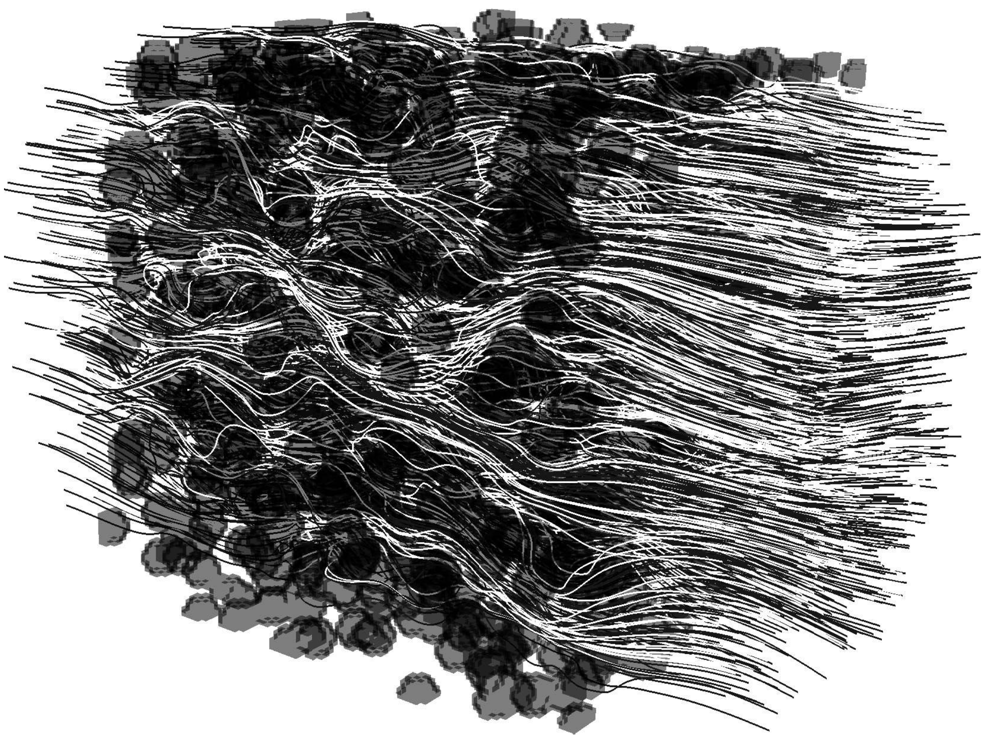


$$\langle \Delta x^2 \rangle = 2 D_{\|} t \ .$$

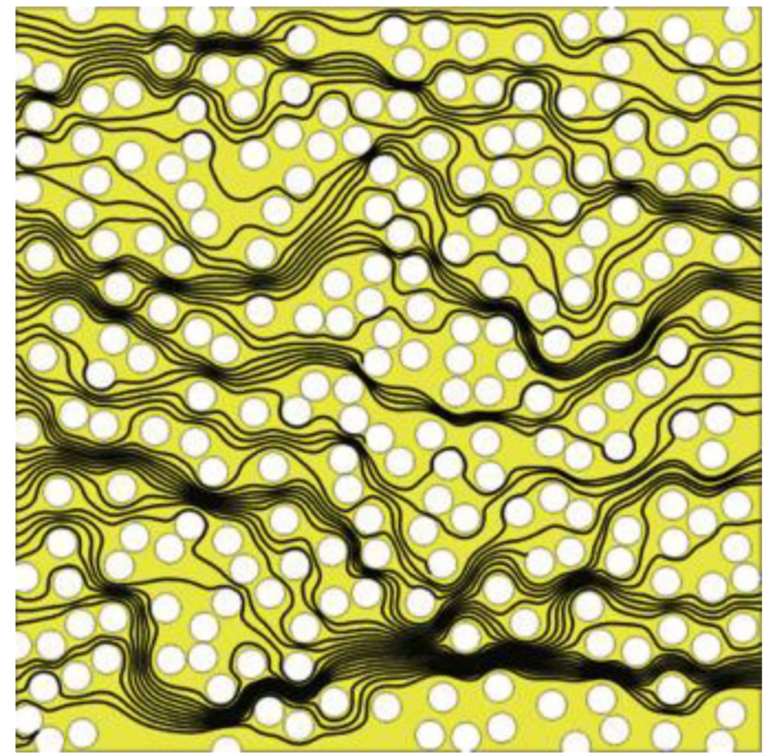
Taylor, G. I. (1953) *Dispersion of soluble matter in solvent flowing slowly through a tube*, Proc. Roy. Soc. A., **219**

Hydrodynamic dispersion

- Generally, the dispersion tensor characterizes the porous medium and the fluids in it



J. Golembiewski

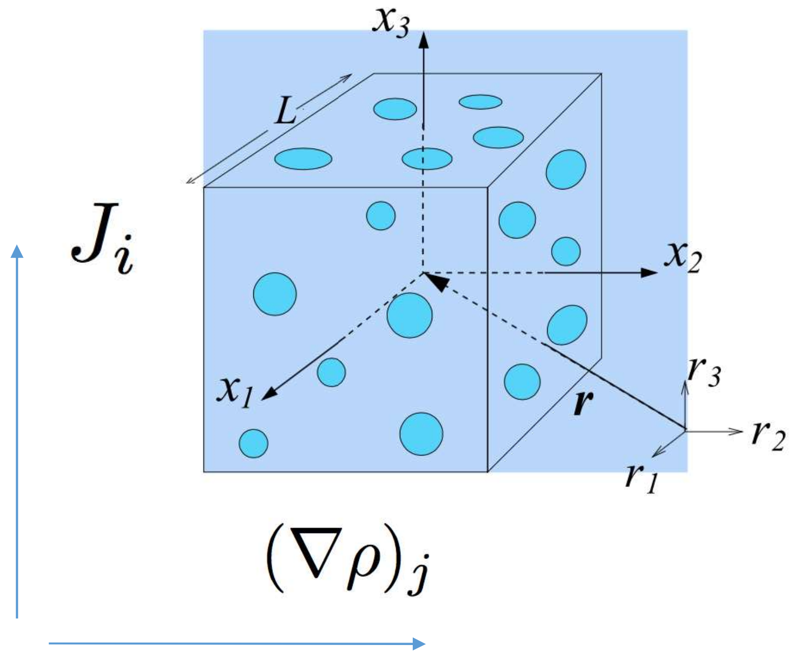


H. Saomoto

What may we say about the dispersion tensor?

- Due to Onsager reciprocity $D_{jk}(\mathbf{u}) = D_{kj}(-\mathbf{u})$

$$\mathbf{J} = \rho_0 \overline{\mathbf{U}} - \mathbf{D} \cdot \nabla \rho_0,$$



Time irreversible equations at the meso-level

- Reversing time does not produce new solutions to the meso-equations

Diffusion equation $\frac{\partial C}{\partial t} = D\nabla^2 C$

Langevin equation $\frac{d\mathbf{v}}{dt} = -\alpha\mathbf{v} + F(t)$ $\langle F(t)F(0)\rangle = A\delta(t)$

$$t \to -t$$

$$\mathbf{v} \to -\mathbf{v}$$

But some meso-equations are reversible still

Particle velocity Given velocity field Fluctuation

Brownian dynamics

$$\mathbf{v} = \mathbf{u}(\mathbf{x}) + \delta\mathbf{v}(t)$$

$$\langle \delta v_i(t) \delta v_j(0) \rangle = A\delta(t)\delta_i$$

Invariant when

$$t \to -t$$
$$\mathbf{v} \to -\mathbf{v}$$
$$\mathbf{u} \to -\mathbf{u}$$

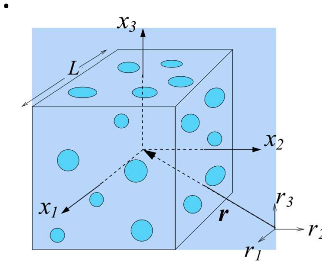
Upon coarse graining above the scale of the mean free path:

Advection diffusion equation

$$\frac{\partial C}{\partial t} + \mathbf{u} \cdot \nabla C = D\nabla^2 C$$

Upon coarse graining on the REV level:

$$\mathbf{J} = \rho_0 \overline{\mathbf{U}} - \mathbf{D} \cdot \nabla \rho_0,$$



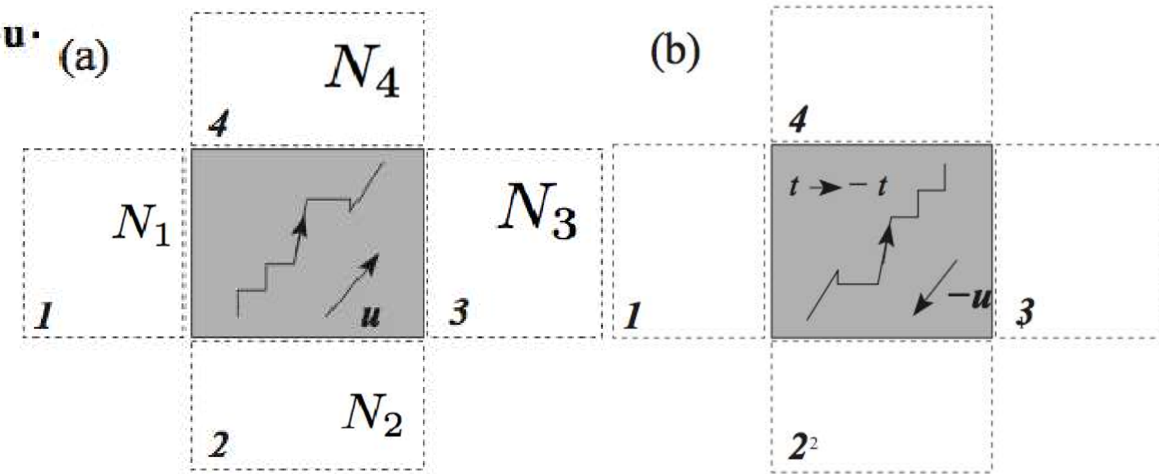
Takes on one value for each REV (representative elementary volume) cell

Time-reversible fluctuations

Reverse the background field ***u*,** then run movie backwards

$$\langle \Delta N_i(\tau)\Delta N_j(0)\rangle_{\mathbf{u}} = \langle \Delta N_i(-\tau)\Delta N_j(0)\rangle_{-\mathbf{u}} = \langle \Delta N_i(0)\Delta N_j(\tau)\rangle_{-\mathbf{u}}$$

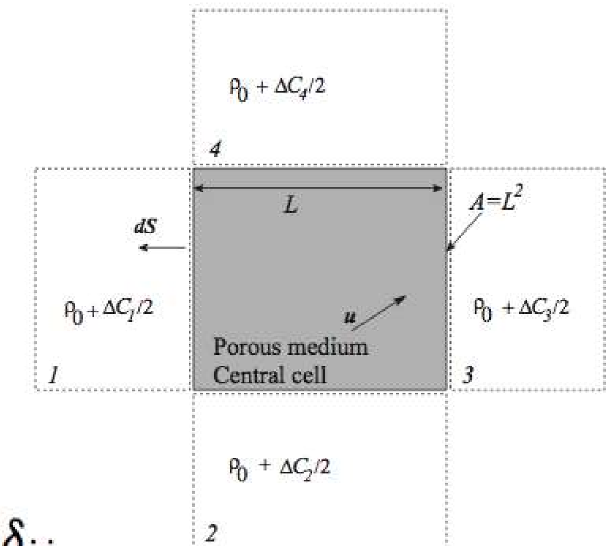
$$\langle \Delta \dot{N}_j \Delta N_k\rangle_{\mathbf{u}} = \langle \Delta \dot{N}_k \Delta N_j\rangle_{-\mathbf{u}}.$$



REV (Representative elementary volume)

Entropy production, fluxes and forces

Entropy production following from standard Gibbs entropy:



$$\sigma = k_B\left(D\frac{(\nabla\rho)^2}{\rho} + \rho\nabla\cdot\mathbf{u}\right).$$

$$\dot{S}_{\rm tot} = \int d^3x\,\sigma = \sum_{i=1}^{2}\frac{\partial S_{\rm tot}}{\partial x_i}\dot{x}_i = \sum_{i=1}^{2}\dot{x}_i F_i,$$

where

$$x_i = \Delta N_i,$$

$$F_i = k_B\frac{\Delta C_i}{\rho_0}.$$

$$P(N_i,\mathbf{u}) \propto \exp[S(N_i,\mathbf{u})/k_B] \longrightarrow \langle x_i F_j\rangle_{\mathbf{u}} = -k_B\delta_{ij}$$

or:

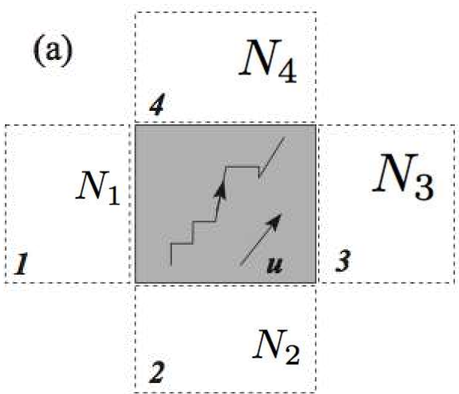
$$\langle \Delta N_i F_j\rangle_{\mathbf{u}} = -k_B\delta_{ij}$$

Relation between the fluctuations and macro-current – the regression hypothesis

$$\langle \Delta \dot{N}_j \Delta N_k \rangle_{\mathbf{u}} = \langle \Delta \dot{N}_k \Delta N_j \rangle_{-\mathbf{u}}$$

$$\mathbf{J} = \rho_0 \overline{\mathbf{U}} - \mathbf{D} \cdot \nabla \rho_0, \qquad \Delta \dot{N}_i = A\left(\rho_o \overline{\mathbf{U}} - D_{ij} \frac{\rho_0}{k_B L} F_j \right).$$

(a)



$$(\nabla \rho_0)_i = \frac{\Delta C_i}{L} = \rho_0 F_i / (k_B L)$$

$$\langle \Delta N_i F_j \rangle_{\mathbf{u}} = -k_B \delta_{ij}$$

$$D_{jk}(\mathbf{u}) = D_{kj}(-\mathbf{u})$$

J.-L. Auriault, C. Moyne, and H. A. Souto, Transp. Porous Med. **85**, 771 (2010).

Other Onsager symmetries include

- Soret effect (temperature and concentration gradients)
- Peltier effect (temperature and electric potential gradients)

FEBRUARY 15, 1931 *PHYSICAL REVIEW* *VOLUME 37*

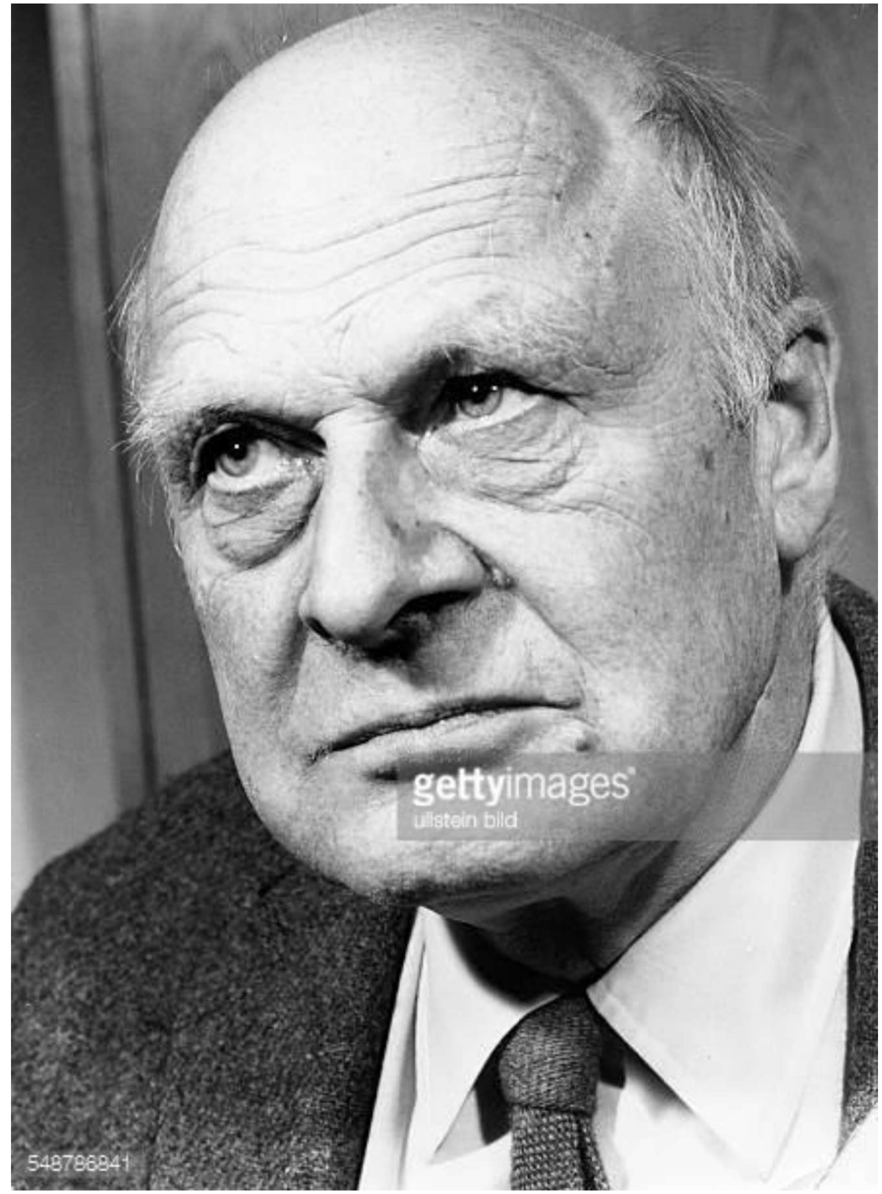
RECIPROCAL RELATIONS IN IRREVERSIBLE PROCESSES. I.

BY LARS ONSAGER
DEPARTMENT OF CHEMISTRY, BROWN UNIVERSITY

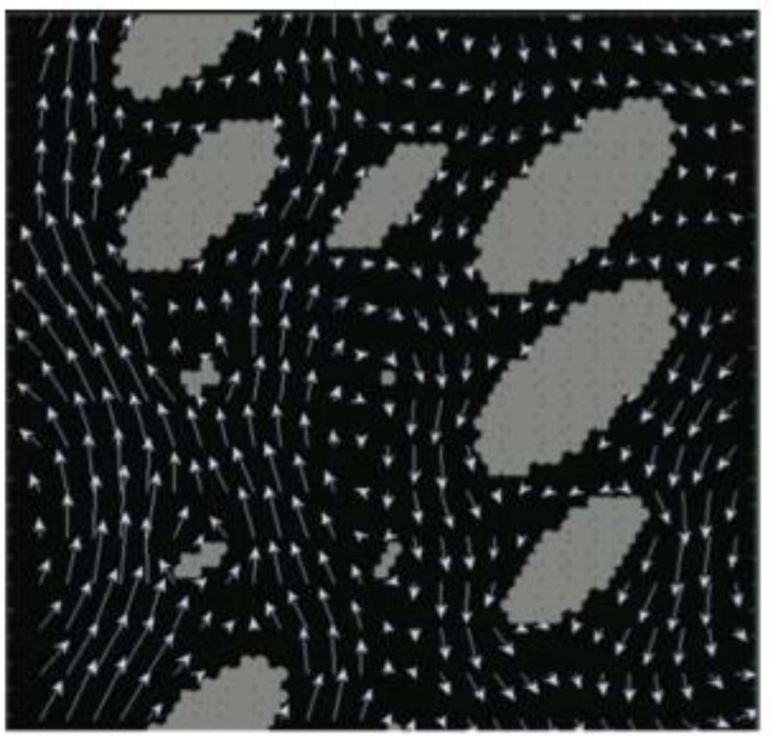
(Received December 8, 1930)

ABSTRACT

Examples of coupled irreversible processes like the thermoelectric phenomena, the transference phenomena in electrolytes and heat conduction in an anisotropic medium are considered. For certain cases of such interaction reciprocal relations have been deduced by earlier writers, e.g., Thomson's theory of thermoelectric phenomena and Helmholtz' theory for the e.m.f. of electrolytic cells with liquid junction. These earlier derivations may be classed as quasi-thermodynamic; in fact, Thomson himself pointed out that his argument was incomplete, and that his relation ought to be established on an experimental basis. A general class of such relations will be derived by a new

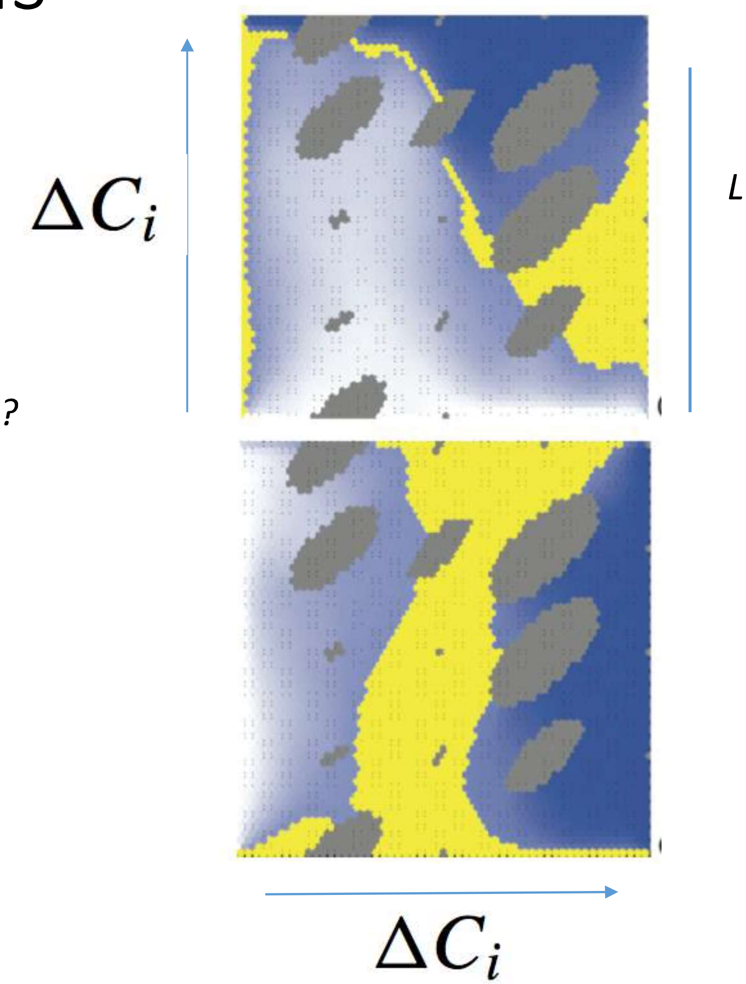


Lattice Boltzmann simulations



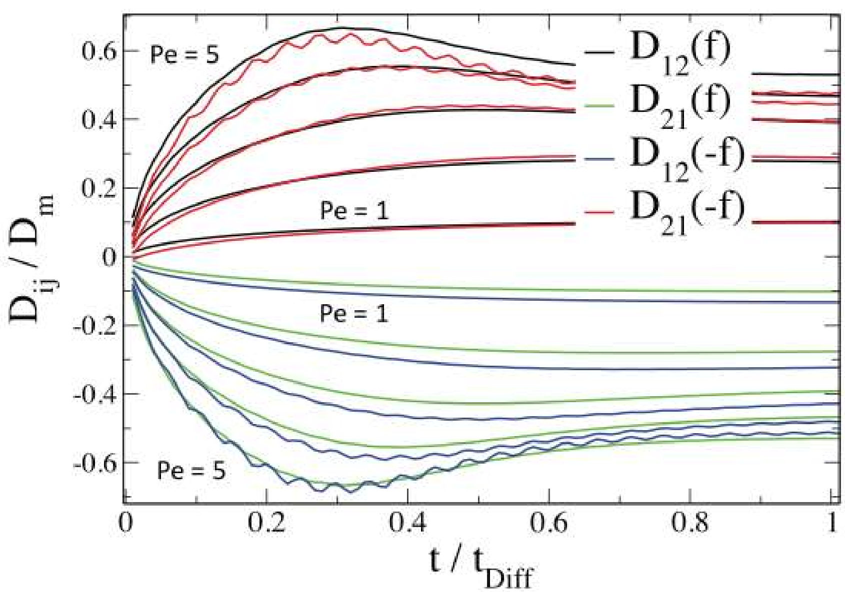
$$D_{jk}(\mathbf{u}) = D_{kj}(-\mathbf{u}) \quad ?$$

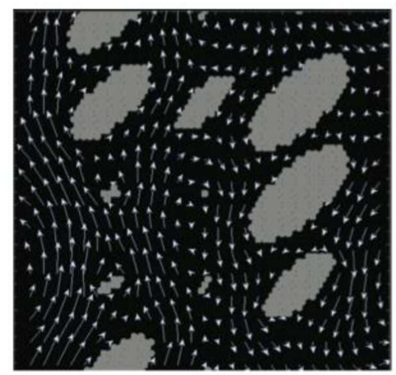
$$D_{jk}(\mathbf{u}) = \frac{J_j}{\Delta C_k / L}$$

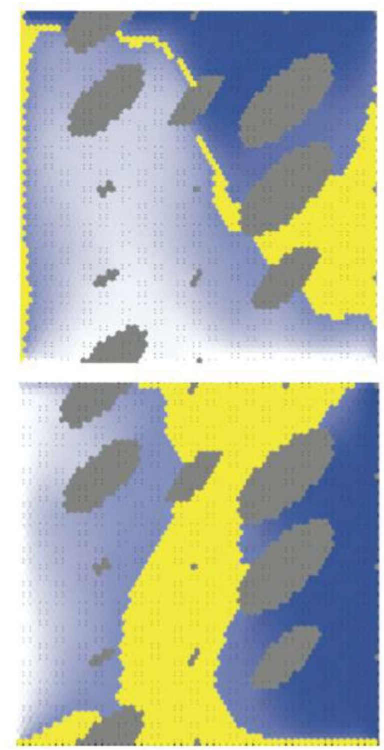


Cross-coupling at various Pe-numbers

Off- diagonal terms depend on flow gradients:







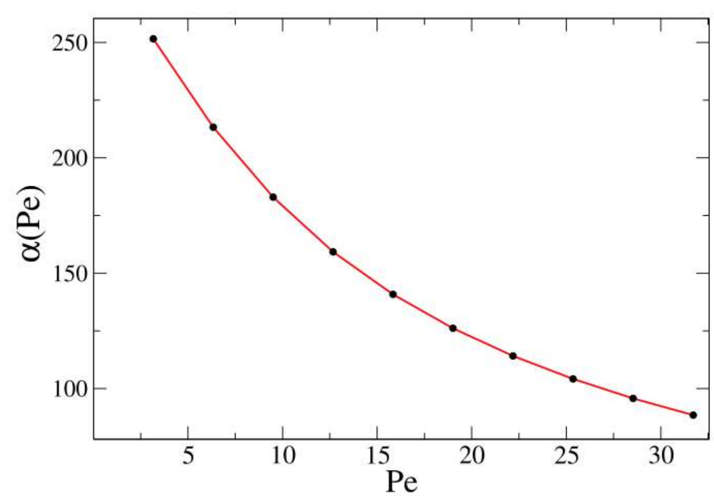
Analytic forms of the dispersion tensor

Off- diagonal terms depend on flow gradients:

$$\mathbf{D} \approx \mathbf{D}^{st} \equiv \frac{D_m}{F}\mathbf{I} + \gamma_l \frac{|\mathbf{q}|}{\phi}\hat{\mathbf{x}}_q\hat{\mathbf{x}}_q + \gamma_t \frac{|\mathbf{q}|}{\phi}(\mathbf{I} - \hat{\mathbf{x}}_q\hat{\mathbf{x}}_q) + \alpha[\nabla\mathbf{q} - (\nabla\mathbf{q})^T]$$

where

$$\hat{\mathbf{x}}_q = \frac{\mathbf{q}}{|\mathbf{q}|}$$



A. E. Scheidegger, J. Geophys. Res. **66**, 3273 (1961).
J. Bear, J. Geophys. Res. **66**, 1185 (1961).
J. Bear, *Dynamics of Fluids in Porous Media* (American Elsevier, New York, 1965).

Conclusions

- Echo dispersion allows both focusing and prediction – a potential medical tool?

- Onsager symmetries can be derived from reversibility at the meso-level as well as the micro-level

- Lattice Boltzmann simulations confirm the predicted symmetry and provides an estimate on a new dispersion tensor

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PHYSICAL REVIEW E **95**, 043103 (2017)
PHYSICAL REVIEW E **95**, 022136 (2017)

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The Research Council of Norway

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UiO : University of Oslo

Thanks, and .... Happy birthday

22.08.2019

Time reversible equations of the micro-world

- Reversing time produces new solutions to the basic equations

$$
\begin{aligned}
t &\to -t \\
q_i(t) &\to q_i(-t) \\
p_i(t) &\to -p_i(-t) \\
\dot{q}_i &\to -\dot{q}_i \\
\mathbf{E} &\to \mathbf{E} \\
\mathbf{B} &\to -\mathbf{B} \\
\mathbf{A} &\to -\mathbf{A} \\
\mathbf{j} &\to -\mathbf{j} \\
\rho &\to \rho
\end{aligned}
$$

$$\psi(t) \to \psi^*(-t) \text{ which means } |\psi(t)|^2 \to |\psi(-t)|^2$$

Hamiltons equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$
$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

Maxwells equations

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}$$
$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \mu_0 \epsilon_0 \frac{\partial \mathbf{E}}{\partial t}$$

Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \left(\frac{1}{2m}(-i\hbar\nabla - \mathbf{A})^2 + \phi \right) \psi$$