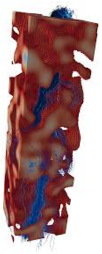
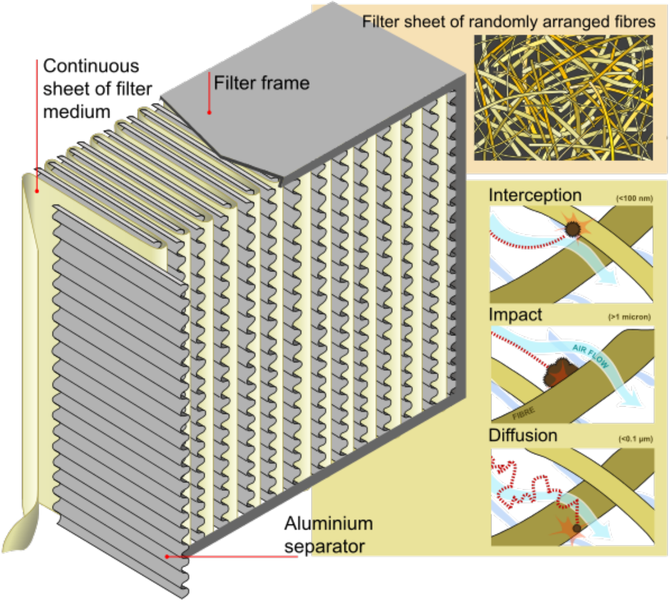


Dispersion and diffusion in porous media

Olivier Liot Petit

Mass transport in porous media: filtration



Take your device

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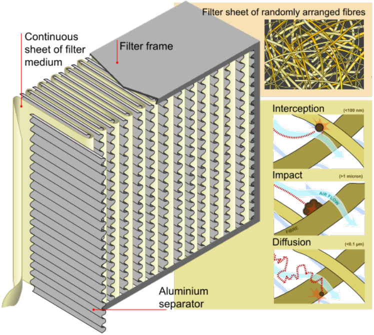


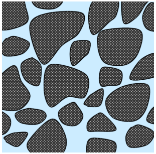
In your opinion, what is the most efficient way of dispersion in a porous media?

A. Advection by the fluid
B. Molecular diffusion
C. Mechanical dispersion due to porous structure
D. It depends on the Péclet number

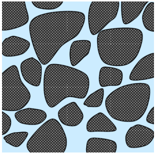
Motivations

Observations:

- Several way of transport
- Interactions fluid/porous structure
- Interactions solute/porous structure



What are the phenomena/parameters which drive the dispersion in a porous media?



Dispersion and diffusion in porous media:

A. **Derivation of the advection-diffusion equation in porous media**

B. **Dispersion mehcanisms**

Objectives of this lecture's section

Dispersion and diffusion in porous media

At the end of these lectures, you should be able to:

- name the different kind of dispersion mechanisms in a porous media
- write and apply the Fick's law
- demonstrate the Taylor's dispersion in a cylinder
- describe diffusion phenomenon in porous media
- write and interpret the advection-dispersion equation
- cite and describe some applications of dispersion in porous media

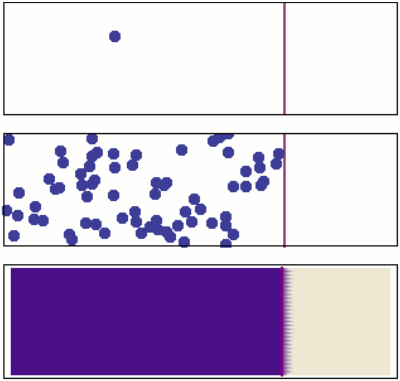
Diffusion in homogeneous media: Fick's law

- Diffusive, stationary flux
- Flux from high concentrations to low concentrations

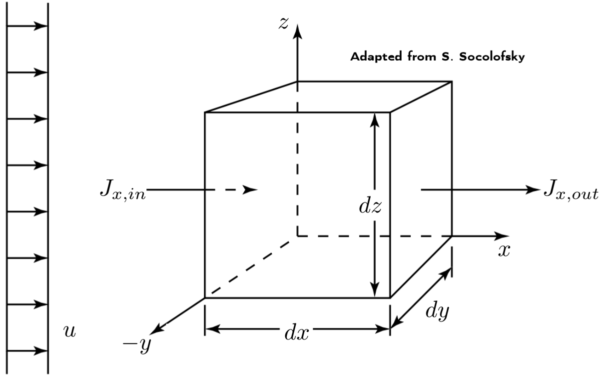
Fick's law

$$\overrightarrow{q} = -D_m \overrightarrow{\mathrm{grad}} \phi$$

- D_m: molecular diffusivity [m^2/s]
- $\overrightarrow{q}$: flux density vector
- ϕ: intensive physical quantity



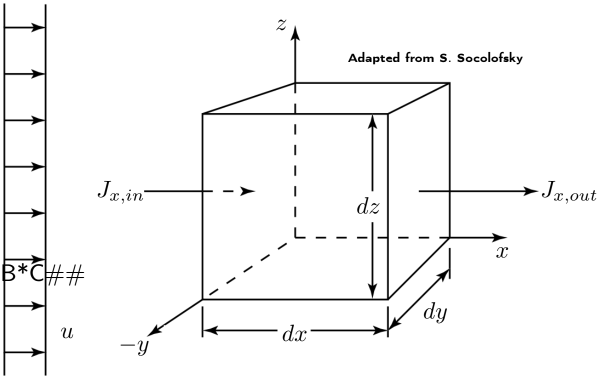
- Diffusivity can be affected by walls $\Rightarrow$ anisotropic diffusion



Exercise: computation of the advection-dispersion equation

Take your device

Advection-dispersion equation



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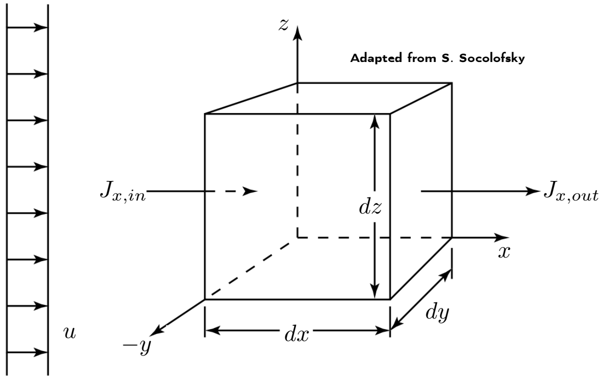
Exercise: computation of the advection-dispersion equation

The advection-dispersion equation is...

A. $\dfrac{\partial C}{\partial t} = \mathrm{div}(D_m \overrightarrow{\mathrm{grad}} C) - \overrightarrow{v} \cdot \overrightarrow{\mathrm{grad}} C$

B. $\dfrac{\partial C}{\partial t} = \mathrm{div}(D_m \overrightarrow{\mathrm{grad}} C) - \mathrm{div}(\overrightarrow{v} C)$

C. $\dfrac{\partial C}{\partial t} = D_m \mathrm{div}(\overrightarrow{\mathrm{grad}} C) - \mathrm{div}(\overrightarrow{v} C)$



Exercise: computation of the advection-dispersion equation

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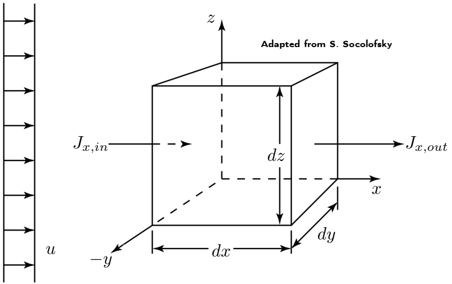
Advection-dispersion equation



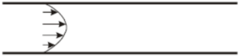
Advection-diffusion equation (no source)

$$\frac{\partial C}{\partial t} = \mathrm{div}(D_m \overrightarrow{\mathrm{grad}} C) - \mathrm{div}(\vec{v}\, C)$$

- c: variable of interest (concentration, temperature...)
- D_m: molecular diffusivity [m^2/s]

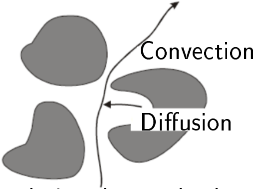
- Related to molecular/particle diffusion
- Related to flow convection

- In porous media: several dispersion mechanisms

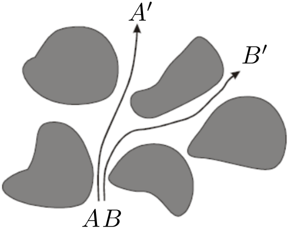


Taylor dispersion

Adapted from M. Quintard

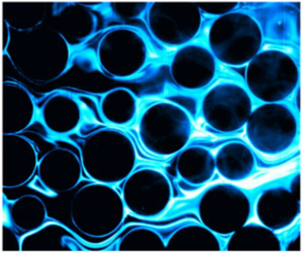


Retardation due to dead-end pores and **tortuosity**



Mechanical dispersion

Volume-averaged advection-dispersion equation



Advection-diffusion equation in a porous media

$$\epsilon \frac{\partial \langle C \rangle^{\alpha}}{\partial t} = \epsilon \mathrm{div}(\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}} \langle C \rangle^{\alpha}) - \mathrm{div}(\langle \overrightarrow{v} \rangle \langle C \rangle^{\alpha})$$

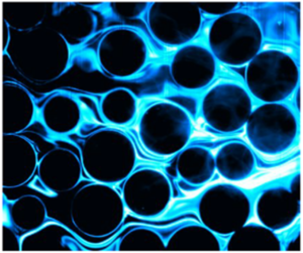
> $\langle C \rangle^{\alpha}$: intrinsic average of solute concentration

> $\overline{\overline{D}}$: effective diffusion/dispersion tensor

> Related to molecular/particle diffusion

> Related to flow convection

Volume-averaged advection-dispersion equation



Advection-diffusion equation in a porous media

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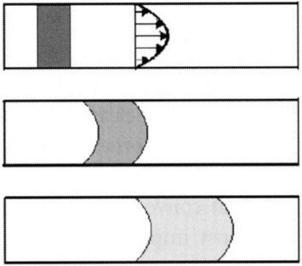
- $\langle C\rangle^{\alpha}$: intrinsic average of solute concentration
- $\overline{\overline{D}}$: effective diffusion/dispersion tensor

- Related to molecular/particle diffusion
- Related to flow convection

What does contain $\overline{\overline{D}}$?

> Due to velocity profile in pores

In a straight pipe:

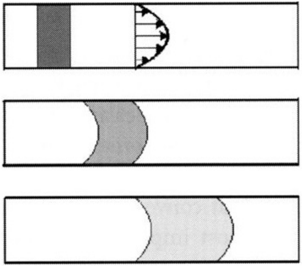


Advection-dispersion equation

$$\frac{\partial C}{\partial t} + v(r)\frac{\partial C}{\partial z} = D_m \Delta C = D_m \left(\frac{\partial^2 C}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial C}{\partial r} \right) \right)$$

> Due to velocity profile in pores

In a straight pipe:



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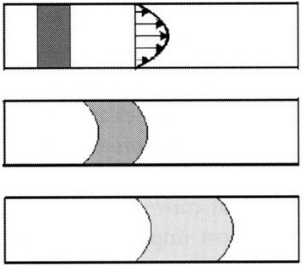
> $C(r,z,t) = \bar{C}(z,t) + C'(r,z,t)$

Dispersion in porous media: Taylor dispersion

> Due to velocity profile in pores

In a straight pipe:



Advection-dispersion equation

$$\frac{\partial C}{\partial t} + v(r)\frac{\partial C}{\partial z} = D_m \Delta C = D_m \left(\frac{\partial^2 C}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial C}{\partial r} \right) \right)$$

> $C(r,z,t) = \bar{C}(z,t) + C'(r,z,t)$

Advection-dispersion equation on average of C

$$\frac{\partial \bar{C}}{\partial t} + \bar{v}\frac{\partial \bar{C}}{\partial z} = D_{eff}\frac{\partial^2 \bar{C}}{\partial z^2}$$

> $D_{eff} = D_m \left(1 + \frac{Pe^2}{48} \right)$

> $Pe = \frac{\text{advection}}{\text{diffusion}} = \frac{a\bar{v}}{D_m}$

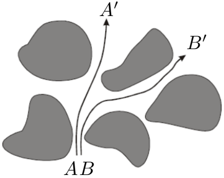
Dispersion in porous media: mechanical dispersion

- Due to porous micro-structure
- Various origins:
  - Mean velocity depends on considered pores
  - Tortuosity
- Separation of particle groups
- Added to Taylor dispersion
- Fick-like dispersion

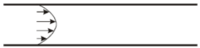
$$\overline{\overline{D}} = \begin{pmatrix} D_{k_{\parallel}} + D_m^{eff} & 0 & 0 \\ 0 & D_{k_{\perp}} + D_m^{eff} & 0 \\ 0 & 0 & D_{k_{\perp}} + D_m^{eff} \end{pmatrix}$$

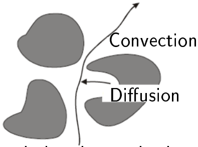
$$\text{with} \begin{cases} D_{k_{\parallel}} = \alpha_{\parallel} ||\langle \overrightarrow{v} \rangle|| \\ D_{k_{\perp}} = \alpha_{\perp} ||\langle \overrightarrow{v} \rangle|| \end{cases} \quad \text{Scheidegger(1951)}$$

- $D_m^{eff} = \dfrac{D_m}{\tau}$: molecular diffusivity corrected by **tortuosity**
- α: dispersivity ($\alpha_{\perp} = \alpha_{\parallel} = \dfrac{a^2 ||\langle \overrightarrow{v} \rangle||}{48 D_m}$ for non-connected cylinder assembly - only T-A)



Mechanical dispersion


Taylor dispersion



Retardation due to dead-end pores and **tortuosity**

Consequence of particle sorption

Remind: advection-diffusion equation (no source)

$$\frac{\partial C}{\partial t} = \mathrm{div}(\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}}\, C) - \mathrm{div}(\overrightarrow{v}\, C)$$

- Adsorption: accumulation of particles at solid/fluid interface
- Chemisorption: integration of elements to the porous structure by chemical reaction

Consequence of particle sorption

Remind: advection-diffusion equation (no source)

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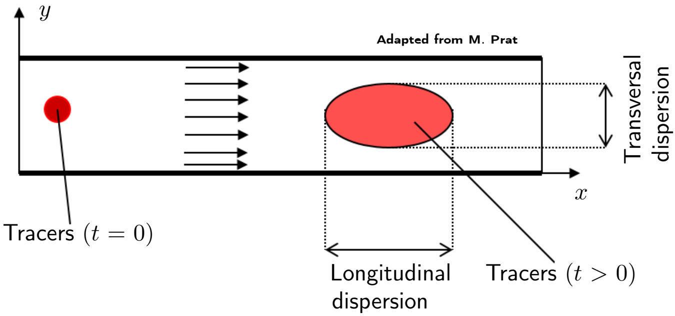
- Adsorption: accumulation of particles at solid/fluid interface
- Chemisorption: integration of elements to the porous structure by chemical reaction
- Source term: $Q_s(C) = -K \dfrac{\partial C}{\partial t}$
- Delay factor: $R = 1 + K$
- Remind: Darcy velocity $\langle \overrightarrow{v} \rangle = \epsilon \langle \overrightarrow{v} \rangle^{\alpha}$; $\langle C \rangle^{\alpha} = \dfrac{1}{V_\alpha} \int_{V_\alpha} C dV$

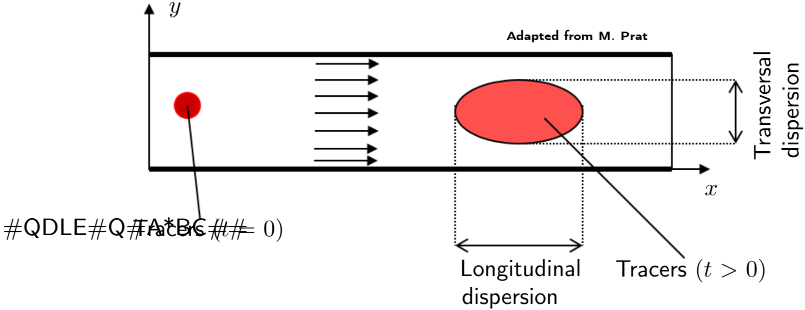
Advection-diffusion equation with sorption in a porous media

$$R\epsilon \frac{\partial \langle C \rangle^{\alpha}}{\partial t} = \epsilon \mathrm{div}(\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}} \langle C \rangle^{\alpha}) - \mathrm{div}(\langle \overrightarrow{v} \rangle \langle C \rangle^{\alpha})$$



Exercise: derivation of the advection-dispersion equation in this case

Take your device



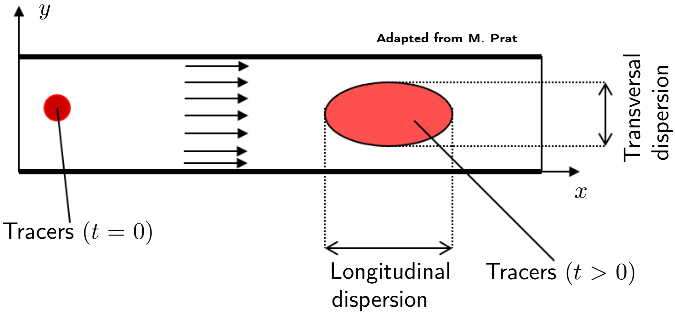
Exercise: derivation of the advection-dispersion equation in this case

The Péclet number expression involving the Darcy velocity is...

A. $Pe = \dfrac{\ell_\alpha \langle \overrightarrow{V} \rangle_x}{\epsilon D_m}$

B. $Pe = \dfrac{\ell_\alpha^2 \langle \overrightarrow{V} \rangle_x}{\epsilon D_m}$

C. $Pe = \dfrac{\epsilon \ell_\alpha \langle \overrightarrow{V} \rangle_x}{D_m}$



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Take your device

And now?

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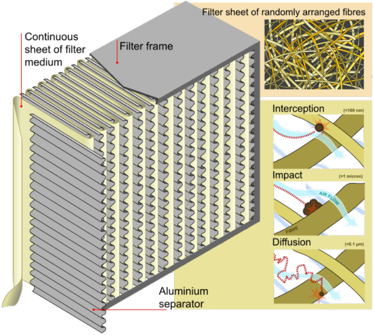
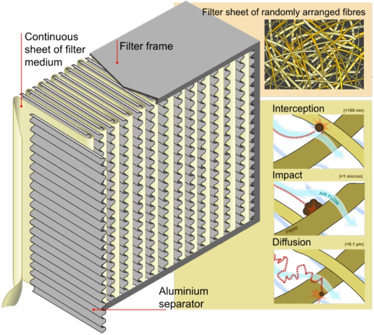


And now, what is the most efficient way of dispersion in a porous media?

A. Advection by the fluid
B. Molecular diffusion
C. Mechanical dispersion due to porous structure
D. It depends on the Péclet number

And now?



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A. Advection by the fluid
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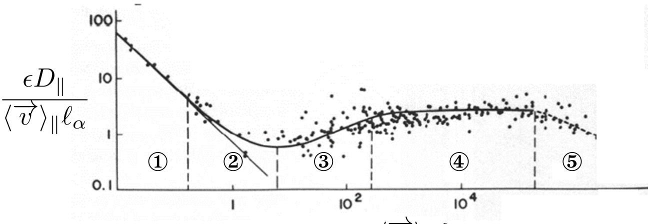
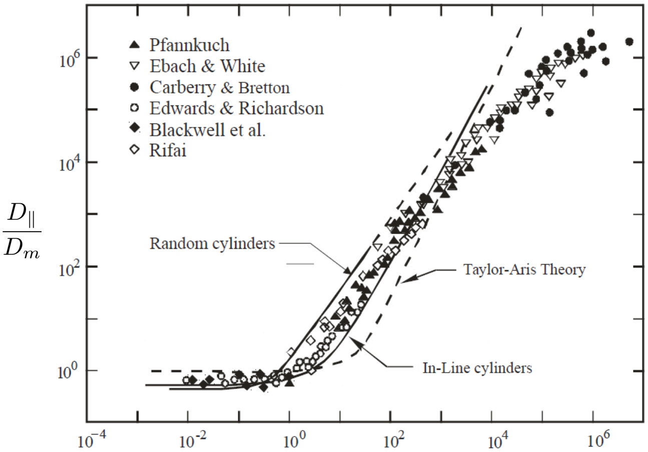
Péclet influence on dispersion



$$Pe = \frac{\langle \overrightarrow{v} \rangle_{\parallel} \ell_{\alpha}}{\epsilon D_m}$$

- ①: only molecular diffusion
- ②: diffusion and mechanical dispersion superposition
- ③: large mechanical dispersion, still molecular diffusion
- ④: only mechanical dispersion
- ⑤: mechanical dispersion with inertia effects

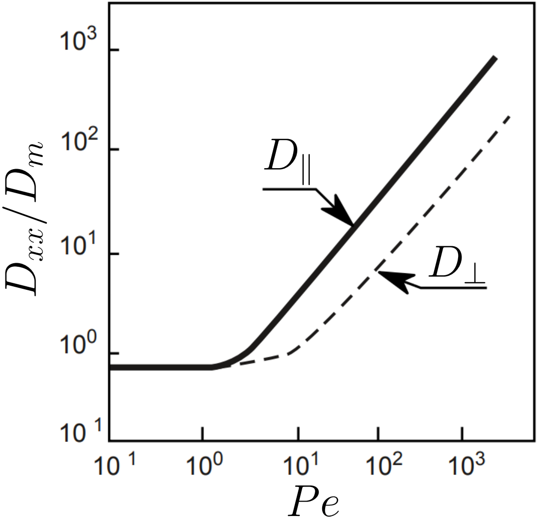
Péclet influence on dispersion



$$Pe = \frac{\langle \overrightarrow{v} \rangle_{\parallel} \ell_{\alpha}}{\epsilon D_m}$$

Péclet influence on dispersion

> Comparison between longitudinal and transverse diffusion coefficients



Adapted from M. Quintard