



Dispersion in Porous Media

Approach by Upscaling

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Journées du GDR MOMAS

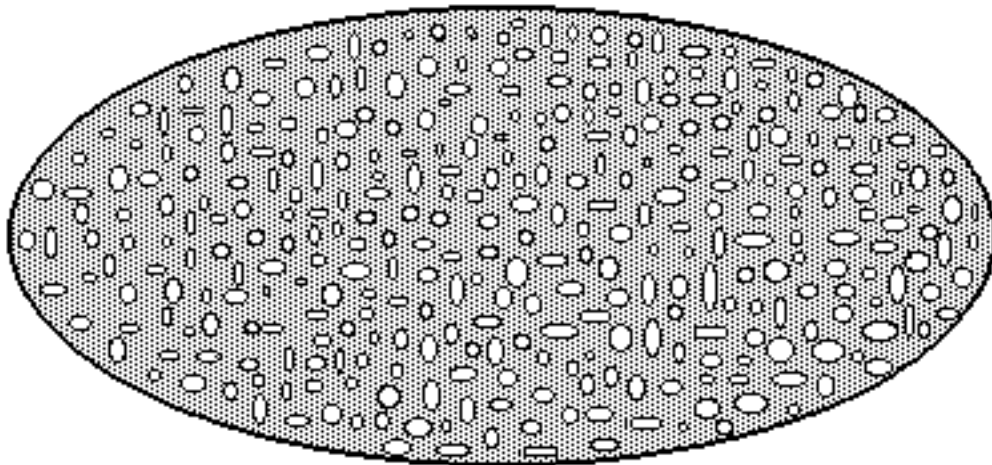
Marseille 28-30 Novembre 2005

Topics

1. Upscaling by multiscale asymptotic expansion technique
2. Darcy's law and its corrector
3. Dispersion in porous media
4. Comments on the validity of the model

1. Upscaling by multiscale asymptotic expansion technique

How to model a heterogeneous media?



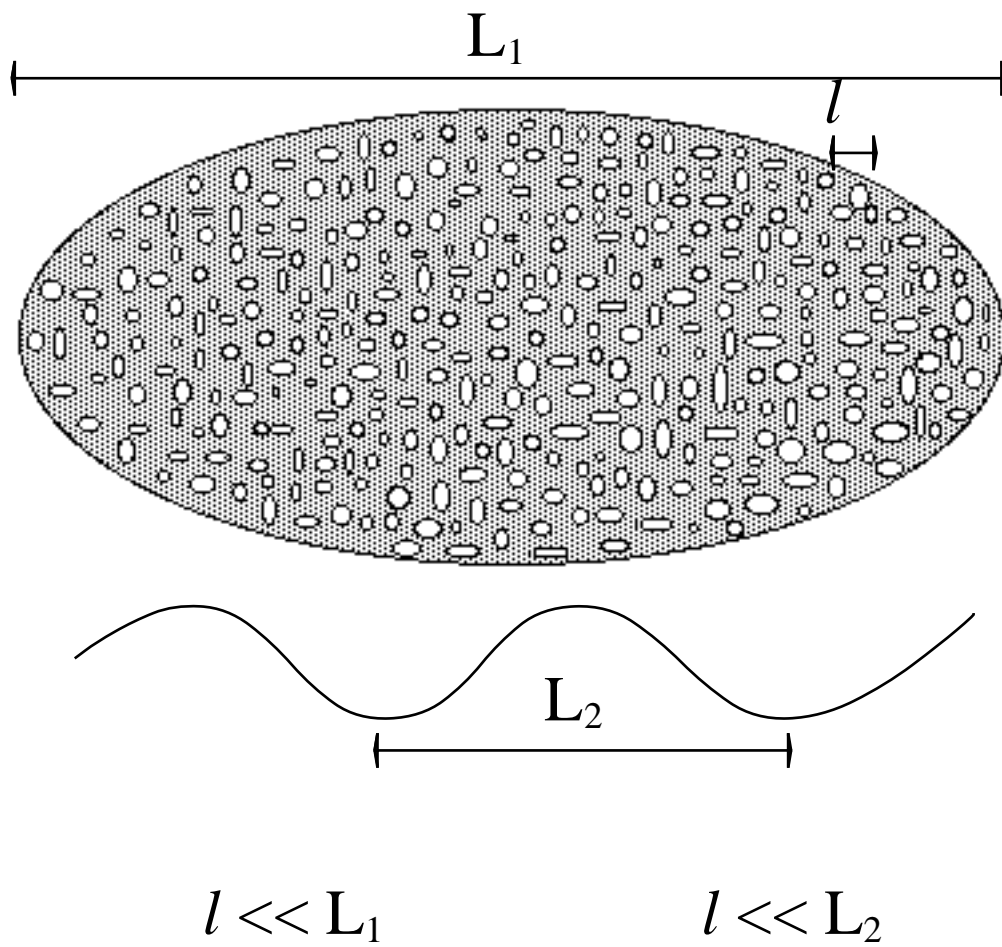
The idea:

Define a continuous medium that is macroscopically equivalent.

The derived macroscopic description must be intrinsic to the material and to the excitation i.e. independent from the macroscopic boundary conditions

Fundamental condition:

The scales must be separated



$$\frac{l}{L} = \varepsilon \ll 1$$

Method of upscaling

**Assumption: the medium is periodic
(No restriction!)**

Method introduced by:

Sanchez-Palencia (1974, 1980)

Keller (1977)

Bensoussan, Lions, Papanicolaou (1980)

J.-L. A. (1991): physical methodology

A. Make dimensionless the heterogeneity scale description

Choose a characteristic length: l or L

$$\phi = \phi_c \phi^*$$

Estimate the dimensionless numbers with respect to ε

$$Q = \mathcal{O}(\varepsilon^p) \quad \text{means} \quad \varepsilon^{p+1} \ll Q \ll \varepsilon^{p-1}$$

Two dimensionless space variables are present

$$\mathbf{x} = \frac{\mathbf{X}}{L}, \quad \mathbf{y} = \frac{\mathbf{X}}{l}$$

B. Introduce asymptotic expansions for the dimensionless unknowns

$$\begin{aligned}\phi^*(\mathbf{y}, \mathbf{x}, t^*) &= \phi^{*0}(\mathbf{x}, \mathbf{y}, t^*) + \varepsilon \phi^{*1}(\mathbf{x}, \mathbf{y}, t^*) \\ &\quad + \varepsilon^2 \phi^{*(2)}(\mathbf{x}, \mathbf{y}, t^*) + \dots\end{aligned}$$

where the ϕ^{*i} are \mathbf{y} -periodic

Extract boundary value problems on the period at the successive orders

Investigate these boundary value problems

C. Macroscopic equivalent model

At a given order, the boundary value problem shows an equation of the form

$$\mathbf{div}_y(\varphi^{*i+1}) + \mathbf{div}_x(\varphi^{*i}) = S^{*i}$$

The existence of a solution imposes a compatibility condition

$$\mathbf{div}_x(\langle \varphi^{*i} \rangle) = \langle S^{*i} \rangle$$

$$\langle \varphi^{*i} \rangle = \int_{\Omega^*} \varphi^{*i} \mathbf{d}y$$

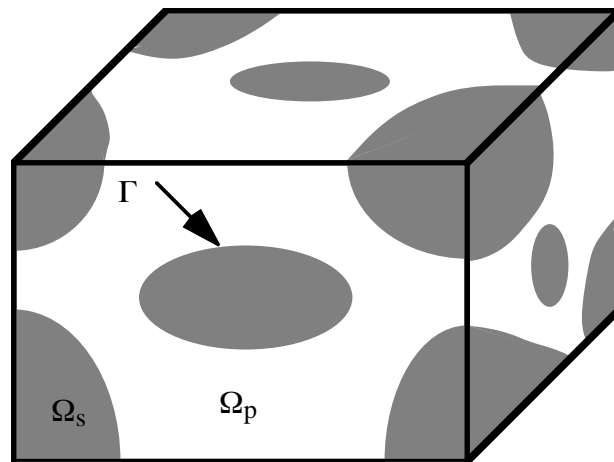
which is a macroscopic description (y is absent)

The compatibility condition for ϕ^{*0} represents the first order approximation of the macroscopic model.

Correctors can be obtained by investigating the following orders

2. Darcy's law and its first corrector

JLA, C. Geindreau, C. Boutin, TIPM
2005



Flow at the pore scale

$$\frac{|\Omega_p|}{|\Omega_s|} = \mathcal{O}(1)$$

Stokes equation

$$\mu \frac{\partial^2 v_i}{\partial X_j \partial X_j} - \frac{\partial p}{\partial X_i} = 0 \quad \mathbf{in} \quad \Omega_p$$

Incompressibility

$$\frac{\partial v_i}{\partial X_i} = 0 \quad \mathbf{in} \quad \Omega_p$$

Adherence condition

$$v_i = 0 \quad \mathbf{on} \quad \Gamma$$

Dimensionless number

$$Q_l = \frac{\left| \frac{\partial p}{\partial X_i} \right|}{\left| \mu \frac{\partial^2 v_i}{\partial X_j \partial X_j} \right|} = \frac{p_c l}{\mu_c v_c}$$

Viscous forces equilibrate pressure forces

$$\frac{\mu_c v_c}{l^2} = \mathcal{O}\left(\frac{p_c}{L}\right) \quad \text{then} \quad Q_l = \mathcal{O}(\varepsilon^{-1})$$

Dimensionless pore scale description

$$\begin{aligned} \mu^* \frac{\partial^2 v_i^*}{\partial y_j \partial y_j} - \varepsilon^{-1} \frac{\partial p^*}{\partial y_i} &= 0 \quad \text{in} \quad \Omega_p^* \\ \frac{\partial v_i^*}{\partial y_i} &= 0 \quad \text{in} \quad \Omega_p^* \\ v_i^* &= 0 \quad \text{on} \quad \Gamma^* \end{aligned}$$

Upscaling process

Introduction of two independent dimensionless space variables

X Physical space variable

$y = \frac{X}{l}$ Microscopic nondimensional space variable

$x = \frac{X}{L} = \varepsilon y$ Microscopic nondimensional space variable

\mathbf{v}^* and p^* are looked for in the form of asymptotic expansions in power of ε

$$\mathbf{v}^* = \mathbf{v}^{*0} + \varepsilon \mathbf{v}^{*1} + \varepsilon^2 \mathbf{v}^{*2} + \dots$$

$$p^* = p^{*0} + \varepsilon p^{*1} + \varepsilon^2 p^{*2} + \dots$$

where functions \mathbf{v}^{*i} and p^{*i} are y -periodic.

Darcy's law (Ene and Sanchez-Palencia, J. de Mcanique 1975)

At the first order the pressure verifies

$$\frac{\partial p^{*0}}{\partial y_i} = 0 \quad \text{then} \quad p^{*0} = p^{*0}(\mathbf{x})$$

The boundary value problem for \mathbf{v}^{*0} and p^{*1} is

$$\mu^* \frac{\partial^2 v_i^{*0}}{\partial y_j \partial y_j} - \frac{\partial p^{*1}}{\partial y_i} - \frac{\partial p^{*0}}{\partial x_i} = 0 \quad \text{in} \quad \Omega_p^*$$

$$\frac{\partial v_i^{*0}}{\partial y_i} = 0 \quad \text{in} \quad \Omega_p^*$$

$$v_i^{*0} = 0 \quad \text{on} \quad \Gamma^*$$

where \mathbf{v}^{*0} and p^{*1} are y-periodic

The pore scale fields are in the form

$$v_i^{*0} = -\frac{k_{ij}^*(\mathbf{x}, \mathbf{y})}{\mu^*} \frac{\partial p^{*0}}{\partial x_i}$$

$$p^{*1} = -\frac{a_i^*(\mathbf{x}, \mathbf{y})}{\mu^*} \frac{\partial p^{*0}}{\partial x_i} + \bar{p}^{*1}(\mathbf{x}), \quad \langle a_i^* \rangle = 0$$

The volume balance

$$\frac{\partial v_i^{*1}}{\partial y_i} + \frac{\partial v_i^{*0}}{\partial x_i} = 0$$

introduces a compatibility condition which is obtained by volume integration

$$\frac{\partial \langle v_i^{*0} \rangle}{\partial x_i} = 0, \quad \langle v_i^{*0} \rangle = -\frac{K_{ij}^*(\mathbf{x})}{\mu^*} \frac{\partial p^{*0}}{\partial x_i},$$

$$\langle v_i^{*0} \rangle = \frac{1}{\Omega_p^*} \int_{\Omega_p^*} v_i^{*0} \mathbf{d}V^*, \quad K_{ij}^* = \frac{1}{\Omega_p^*} \int_{\Omega_p^*} k_{ij}^* \mathbf{d}V^*$$

$\langle \mathbf{v}^{*0} \rangle$ is a flux

At the first order of approximation, the flow is described by a "Darcy's law" and an incompressibility condition

$$\langle v_i \rangle = -\frac{K_{ij}(\mathbf{X})}{\mu} \frac{\partial p}{\partial X_i} + \mathcal{O}(\varepsilon \langle v_i \rangle),$$

$$\frac{\partial \langle v_i \rangle}{\partial X_i} = \mathcal{O}(\varepsilon \frac{\partial \langle v_i \rangle}{\partial X_i}), \quad K_{ij} = l^2 K_{ij}^*$$

First corrector

The boundary value problem for \mathbf{v}^{*1} and p^{*2} is

$$\begin{aligned} \mu^* \frac{\partial^2 v_i^{*1}}{\partial y_j \partial y_j} + 2\mu^* \frac{\partial^2 v_i^{*0}}{\partial y_j \partial x_j} - \frac{\partial p^{*2}}{\partial y_i} - \frac{\partial p^{*1}}{\partial x_i} &= 0 \quad \text{in } \Omega_p^* \\ \frac{\partial v_i^{*1}}{\partial y_i} + \frac{\partial v_i^{*0}}{\partial x_i} &= 0 \quad \text{in } \Omega_p^* \\ v_i^{*1} &= 0 \quad \text{on } \Gamma^* \end{aligned}$$

where \mathbf{v}^{*1} and p^{*2} are y -periodic

The pore scale velocity field \mathbf{v}^{*1} is given by

$$\begin{aligned} v_i^{*1} &= - \frac{k_{ij}^*(\mathbf{x}, \mathbf{y})}{\mu^*} \frac{\partial \bar{p}^{*1}}{\partial x_i} - \frac{l_{ij}^*(\mathbf{x}, \mathbf{y})}{\mu^*} \frac{\partial p^{*0}}{\partial x_i} \\ &\quad - \frac{n_{ijk}^*(\mathbf{x}, \mathbf{y})}{\mu^*} \frac{\partial^2 p^{*0}}{\partial x_j \partial x_k} \end{aligned}$$

The volume balance

$$\frac{\partial v_i^{*2}}{\partial y_i} + \frac{\partial v_i^{*1}}{\partial x_i} = 0$$

introduces a compatibility condition which is obtained by volume integration

$$\frac{\partial \langle v_i^{*1} \rangle}{\partial x_i} = 0,$$

$$\langle v_i^{*1} \rangle = -\frac{K_{ij}^*(\mathbf{x})}{\mu^*} \frac{\partial \bar{p}^{*1}}{\partial x_i} - \frac{L_{ij}^*(\mathbf{x})}{\mu^*} \frac{\partial p^{*0}}{\partial x_i} - \frac{N_{ijk}^*(\mathbf{x})}{\mu^*} \frac{\partial^2 p^{*0}}{\partial x_j \partial x_k},$$

$$L_{ij}^* = \langle l_{ij}^* \rangle, \quad N_{ijk}^* = \langle n_{ijk}^* \rangle$$

$\langle \mathbf{v}^{*1} \rangle$ is generally not a flux

In the dimensional form

$$\langle v_i^1 \rangle = -\frac{K_{ij}(\mathbf{X})}{\mu} \frac{\partial \bar{p}^1}{\partial X_i} - \frac{L_{ij}(\mathbf{X})}{\mu} \frac{\partial \bar{p}^1}{\partial X_i} - \frac{N_{ij}(\mathbf{X})}{\mu} \frac{\partial^2 p^0}{\partial X_j \partial X_k}$$

$$\frac{\partial \langle v_i^1 \rangle}{\partial X_i} = 0, \quad L_{ij} = l^2 L_{ij}^*, \quad N_{ijk} = l^2 L N_{ij}^*$$

Corrected flow law

Introduce the corrected velocity and pressure

$$\begin{aligned} v_i &\approx v_i^0 + \varepsilon v_i^1 \\ p &\approx p^0 + \varepsilon p^1 \end{aligned}$$

The corrected dimensional flow law takes the form

$$\begin{aligned} \frac{\partial \langle v_i \rangle}{\partial X_i} &= \mathcal{O}\left(\varepsilon \frac{\partial \langle v_i \rangle}{\partial X_i}\right) \\ \langle v_i \rangle &= -\frac{K_{ij} + L_{ij}^{eff}}{\mu} \frac{\partial \langle p \rangle}{\partial X_i} \\ &\quad - \frac{N_{ijk}^{eff}}{\mu} \frac{\partial^2 \langle p \rangle}{\partial X_j \partial X_k} + \mathcal{O}(\varepsilon^2 \langle v_i \rangle) \\ L_{ij}^{eff} &= \mathcal{O}\left(\frac{l^2}{L}\right) \quad N_{ijk}^{eff} = \mathcal{O}(l^3) \end{aligned}$$

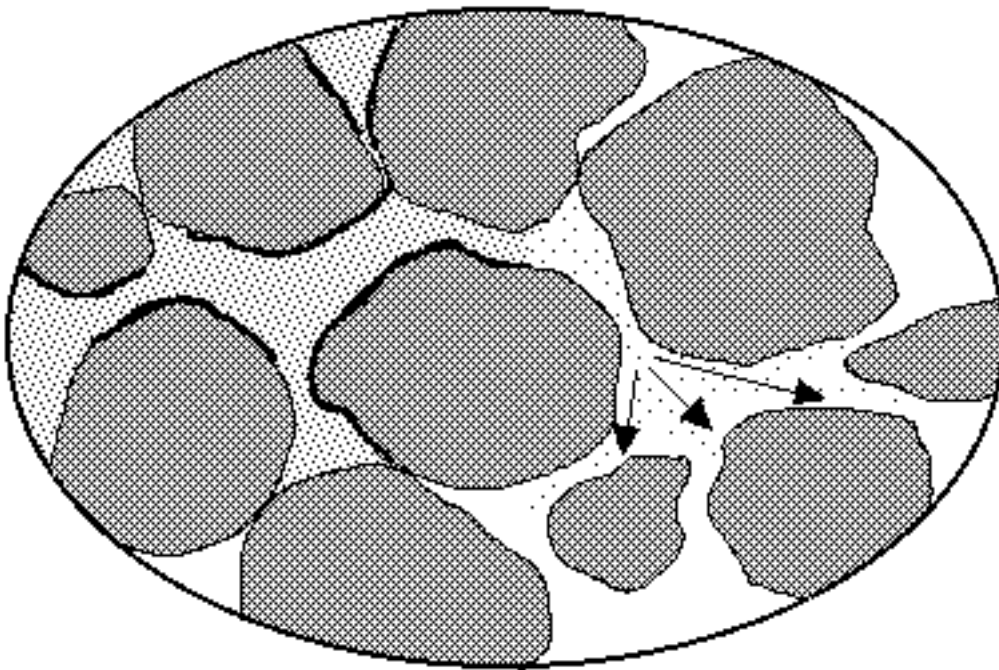
In case of macroscopically homogeneous and isotropic porous media

$$L_{ij}^{eff} = 0, \quad N_{ijk}^{eff} = 0,$$

$\langle \mathbf{v}^{*1} \rangle$ is a flux and the corrected flow law is a Darcy's law!

3. Dispersion in porous media

JLA and P. Adler, ADWR 1995



Diffusion and advection are present

Pore scale description

Isotropic molecular diffusion

$$\frac{\partial c}{\partial t} + \frac{\partial}{\partial X_i} \left(-D \frac{\partial c}{\partial X_i} + v_i c \right) = 0$$

Boundary condition

$$D \frac{\partial c}{\partial X_i} N_i = 0 \quad \text{on} \quad \Gamma$$

Dimensionless local equations

$$\frac{l^2}{D_c t_c} \frac{\partial c^*}{\partial t^*} + \frac{\partial}{\partial y_i} \left(-D^* \frac{\partial c^*}{\partial y_i} + \frac{v_{cl}}{D_c} v_i^* c^* \right) = 0$$

$$D^* \frac{\partial c^*}{\partial y_i} N_i = 0 \quad \text{on} \quad \Gamma^*$$

Dimensionless numbers

$$\mathcal{P}e_l = \frac{\left| \frac{\partial}{\partial X_i} (v_i c) \right|}{\left| \frac{\partial}{\partial X_i} \left(D \frac{\partial c}{\partial X_i} \right) \right|} = \frac{v_{cl}}{D_c} \quad \text{Péclet number}$$

$$\mathcal{P}l = \frac{\left| \frac{\partial c}{\partial t} \right|}{\left| \frac{\partial}{\partial X_i} \left(D \frac{\partial c}{\partial X_i} \right) \right|} = \frac{l^2}{D_c t_c}$$

Characteristic macroscopic times

Characteristic diffusion time

$$T_L^{diff} = \frac{L^2}{D_c}$$

Characteristic advection time

$$T_L^{adv} = \frac{L}{v_c}$$

Different estimations

A. Predominant diffusion at macroscale

Observation time

$$t_c = T_L^{diff} = \varepsilon T_L^{adv} \quad \Longrightarrow \quad \mathcal{P}e_l = \varepsilon^2 \quad \mathcal{P}_l = \varepsilon^2$$

B. Diffusion and advection equivalent at macroscale

Observation time

$$t_c = T_L^{diff} = T_L^{adv} \quad \Longrightarrow \quad \mathcal{P}e_l = \varepsilon \quad \mathcal{P}_l = \varepsilon^2$$

C. Predominant advection at macroscale: dispersion

Observation time

$$t_c = T_L^{adv} = \varepsilon T_L^{diff} \quad \Longrightarrow \quad \mathcal{P}e_l = 1 \quad \mathcal{P}_l = \varepsilon$$

D. Very strong advection at macroscale: non-homogenizable

Observation time

$$t_c = T_L^{adv} = \varepsilon^2 T_L^{diff} \quad \Longrightarrow \quad \mathcal{P}e_l = \varepsilon^{-1} \quad \mathcal{P}_l = 1$$

C. Predominant advection at macroscale: dispersion

$$t_c = T_L^{adv} = \varepsilon T_L^{dif}, \quad \mathcal{P}e_l = 1 \quad \mathcal{P}_l = \varepsilon$$

Local dimensionless description

$$\varepsilon \frac{\partial c^*}{\partial t^*} + \frac{\partial}{\partial y_i} \left(-D^* \frac{\partial c^*}{\partial y_i} + v_i^* c^* \right) = 0$$

$$D^* \frac{\partial c^*}{\partial y_i} N_i = 0 \quad \text{on} \quad \Gamma^*$$

Homogenization process

Boundary value problem for c^{*0}

$$\frac{\partial}{\partial y_i} \left(D^* \frac{\partial c^{*0}}{\partial y_i} - v_i^{*0} c^{*0} \right) = 0$$

$$D^* \frac{\partial c^{*0}}{\partial y_i} N_i = 0 \quad \text{on} \quad \Gamma^*$$

c^{*0} **y**-periodic

Solution

$$c^{*0} = c^{*0}(\mathbf{x}, t^*)$$

Boundary value problem for c^{*1}

$$\frac{\partial}{\partial y_i} \left(D^* \left(\frac{\partial c^{*1}}{\partial y_i} + \frac{\partial c^{*0}}{\partial x_i} \right) - v_i^{*0} c^{*1} - v_i^{*1} c^{*0} \right) - \frac{\partial v_i^{*0} c^{*0}}{\partial x_i} = \frac{\partial c^{*0}}{\partial t^*}$$

$$D^* \left(\frac{\partial c^{*1}}{\partial y_i} + \frac{\partial c^{*0}}{\partial x_i} \right) N_i = 0 \quad \text{on} \quad \Gamma^*$$

c^{*1} y-periodic

Compatibility condition: first order macroscopic behaviour

$$\frac{\partial \langle v_i^{*0} \rangle c^{*0}}{\partial x_i} + \phi \frac{\partial c^{*0}}{\partial t^*} = 0$$

Diffusion is absent.

Let us investigate the first corrector

c^{*1} Solution

$$c^{*1} = \chi_i^*(\mathbf{x}, \mathbf{y}, D^*, \mathbf{grad} p^{*0}) \frac{\partial c^{*0}}{\partial x_i} + \bar{c}^{*1}(\mathbf{x})$$

$$\langle \chi_i^* \rangle = 0$$

χ_i^* depends on D^* and on the advection

Boundary value problem for c^{*2}

$$\begin{aligned} & \frac{\partial}{\partial y_i} \left(D^* \left(\frac{\partial c^{*2}}{\partial y_i} + \frac{\partial c^{*1}}{\partial x_i} \right) - v_i^{*0} c^{*2} - v_i^{*1} c^{*1} - v_i^{*2} c^{*0} \right) \\ & + \frac{\partial}{\partial x_i} \left(D^* \left(\frac{\partial c^{*1}}{\partial y_i} + \frac{\partial c^{*0}}{\partial x_i} \right) - v_i^{*1} c^{*0} - v_i^{*0} c^{*1} \right) = \frac{\partial c^{*1}}{\partial t^*} \end{aligned}$$

$$D^* \left(\frac{\partial c^{*2}}{\partial y_i} + \frac{\partial c^{*1}}{\partial x_i} \right) N_i = 0 \quad \text{on} \quad \Gamma^*$$

c^{*2} y-periodic

The compatibility condition gives the first corrector

$$\begin{aligned} & \frac{\partial}{\partial x_i} \left(D_{ij}^{*disp} \frac{\partial c^{*0}}{\partial x_j} - \langle v_i^{*1} \rangle c^{*0} - \langle v_i^{*0} \rangle \bar{c}^{*1} \right) \\ & = \phi \frac{\partial \bar{c}^{*1}}{\partial t^*} \end{aligned}$$

The $D_{ij}^{*disp}(\mathbf{x}, D^*, \text{grad} p^{*0})$'s are the dispersion tensor components. D^{*disp} is positive non-symmetrical.

Macroscopic model including the corrector

$$c^* \approx c^{*0} + \varepsilon c^{*1} \quad \mathbf{v}^* = \mathbf{v}^{*0} + \varepsilon \mathbf{v}^{*1}$$

Macroscopic dimensionless model

$$\begin{aligned} \frac{\partial}{\partial x_i} \left(\varepsilon D_{ij}^{*disp} \frac{\partial \langle c^* \rangle}{\partial x_i} - \langle v_i^* \rangle \frac{\langle c^* \rangle}{\phi} \right) \\ = \frac{\partial \langle c^* \rangle}{\partial t^*} + \mathcal{O}(\varepsilon^2) \end{aligned}$$

Macroscopic dimensional model

$$\begin{aligned} \frac{\partial}{\partial X_i} \left(D_{ij}^{disp} \frac{\partial \langle c \rangle}{\partial X_i} - \langle v_i \rangle \frac{\langle c \rangle}{\phi} \right) \\ = \frac{\partial \langle c \rangle}{\partial t} + \mathcal{O}\left(\varepsilon^2 \frac{\partial \langle c \rangle}{\partial t}\right) \end{aligned}$$

4. Comments on the validity of the model

Physical meaning of the macroscopic quantities?

Influence of the boundary layers that should be introduced along the macroscopic boundaries?

Is the separation of scales verified in the bulk material?

Physical meaning of the macroscopic quantities

JLA, C. Geindreau and C. Boutin,
TIPM 2005

The problem concerns the macroscopic velocity. Is it a flux?

\mathbf{v}^0 is γ divergence free. Therefore $\langle \mathbf{v}^0 \rangle$ is a flux, i.e. a Darcy velocity.

\mathbf{v}^1 is not γ divergence free. Therefore $\langle \mathbf{v}^1 \rangle$ is not generally a flux
 $\langle \mathbf{v} \rangle \approx \langle \mathbf{v}^0 + \varepsilon \mathbf{v}^1 \rangle$ is not a Darcy velocity.

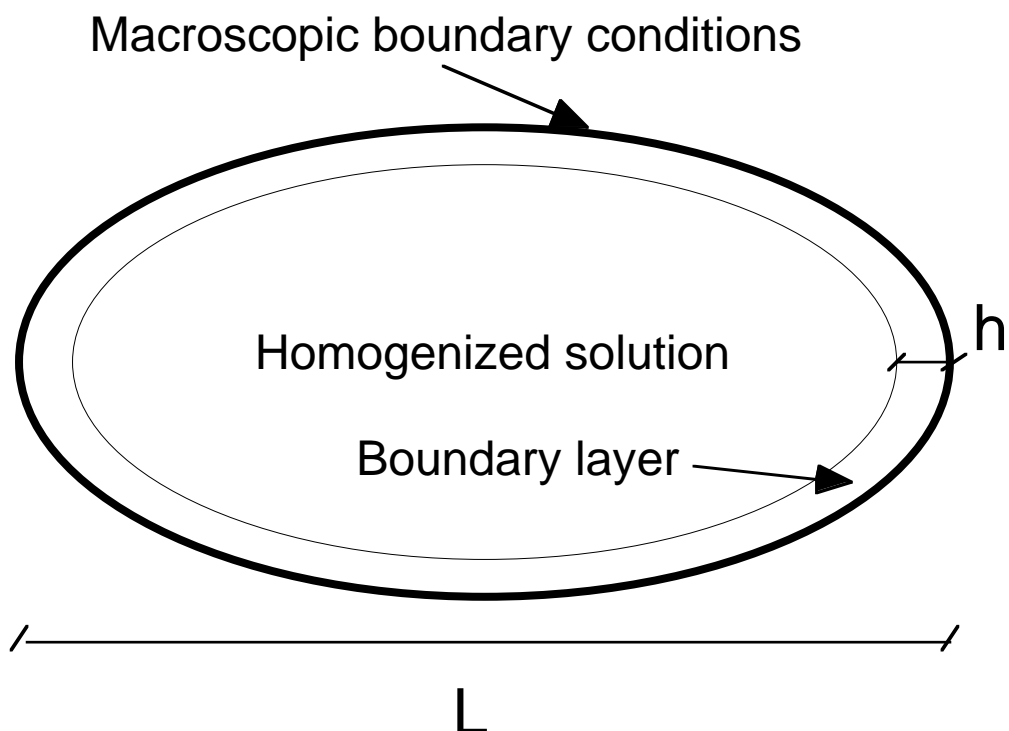
$\langle \mathbf{v} \rangle \approx \langle \mathbf{v}^0 + \varepsilon \mathbf{v}^1 \rangle$ is a Darcy velocity if the porous medium is macroscopically homogeneous and isotropic.

If not Darcy's law is not valid. Modification of the convective term is \mathcal{O} (dispersion term)

Boundary layers

JLA and J. Lewandowska, Engng Trans.
1997

Boundary layers must be introduced to match the homogenised solution to the macroscopic boundary conditions



Purely diffusive transfert

$$h = \mathcal{O}(l)$$

Transit time in the diffusive boundary layer

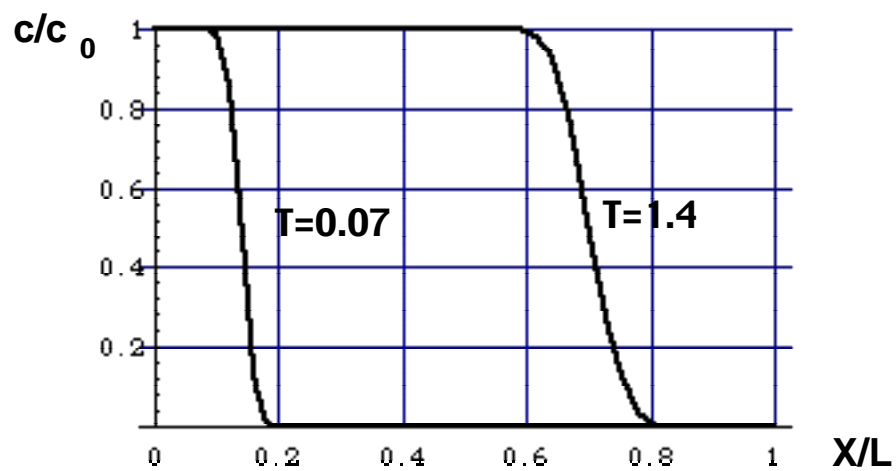
$$T_h^{diff} = \frac{h^2}{D}$$

In case of dispersion, the boundary layer is stretched by convection

$$h^{disp} = v_c T_h^{diff} = \frac{v_c h^2}{D} = h \mathcal{P}e_l$$

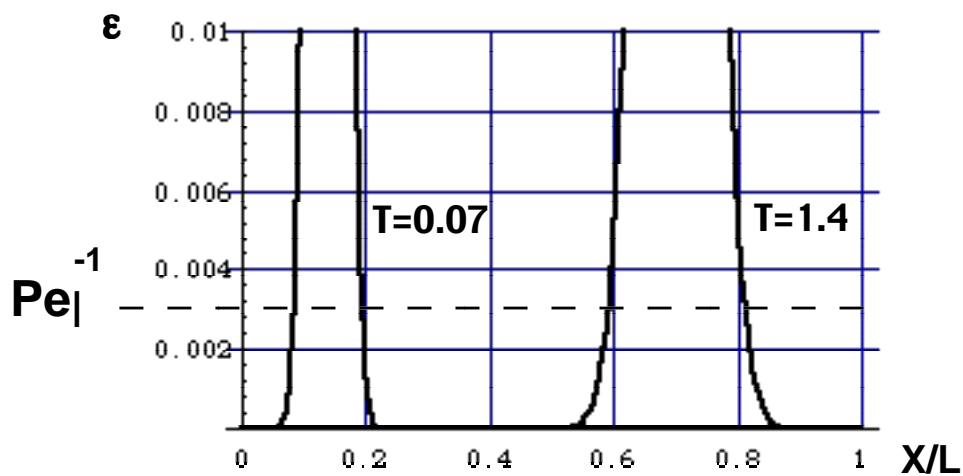
In case of dispersion the boundary layer thickness is much larger

Are scales well separated?



The macroscopic length L is smaller on the wave-front. In this place $\varepsilon = l/L$ is larger and the separation of scales could be poor

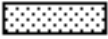


Bues and Aachib experiments, Exp. in Fluids, 1991



Areas where $\varepsilon > 0.1$ are (arbitrarily) said
non-homogenizable

$\mathcal{P}e_l^{-1} = \mathcal{O}(\varepsilon)$ is a non-homogenizable situation



-  dispersion zone: homogenizable zone
-  dispersion zone: non-homogenizable zone
-  advection zone $c=c_0$

5. Conclusion

Darcy's law is robust.

Dispersion law is not robust