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Transfers in Porous Media
– Lecture Notes

This document is a framework for the lecture *Transfers in Porous Media* (MIPO) provided in the MF2E Department (ENSEEIHT) and the FEIP Master (INSA Toulouse/ENSEEIHT). It presents a description of porous media and their properties. The central point of this course concerns upscaling methods which are detailed. Hydrodynamic transport in a porous media is derived as an illustration of these methods. Finally, dispersion in porous media and heat transport are addressed.

This document needs to be red side-to-side with the slides of the lecture and the corresponding exercises, especially in order to illustrate the speech.

Lecture 1

Description of porous media

A lot of natural and artificial objects and situations involve transfers in porous media. A porous media is a material containing a large quantity of pores, 2D or 3D-arranged. They can manage numerous of functions, as illustrated below.

- Wood: hard pores transporting sap;
- Limestone, bricks or rocks: hard but possibly reactive holes where water can infiltrate;
- Cell nucleus or cell surface: hole where macromolecules can by chemical selectively cross the surface;
- Blood vessels: deformable porous network;
- Filter: controlled in size and material pores. Must prevent passage of particles;
- Fibreglass: soft porous media with large calorific capacity, fibrous.

More generally, a porous media is a heteregoneous media where channels, cavities, crevices or orifices cross a solid media or come out on its surface. Pore dimensions can spread on 7 orders of magnitude (from 10^{-4} to more than $10^3\,\mu$m). They can be classified depending on the size (according to International Union of Pure and Applied Chemistry): micro-pores (up to 2 nm), meso-pores (from 2 to 50 nm) and macro-pores (more than 50 nm).

Learning objectives At the end of this lecture, you should be able to:

- describe some natural and artificial porous media
- define and compute the Knudsen number
- define and explain the main properties of a porous media (porosity, tortuosity, saturation)

1.1 Description of porous media

A porous media can have a lot of shapes, topologies, constitutions. It is made of at least two phases (including one solid phase). For example, inside an aquifer, the number of phases can vary depending on the location and physico-chemical conditions. We can encounter water in a solid matrix, an oil+water mixture, a mix of gas and liquid(s). Furthermore, a media can have different porosities at different scales as in a catalysis bed reactor.

Three classes of porous media exist : fibrous, non-consolidated and consolidated (see Slides).

With such a variety of phases or materials, coexistence of scales, how to have a quantitative approach of porous media properties? That will be the guideline of this lecture, in order to get macroscopic properties from microscopic laws.

1.2 Physics at pore scale: Knudsen number

Before upscaling local laws to the porous media scale, we have to be sure that these laxs are still valid at pore scale. For **liquids**, Navier-Stokes and Stokes equation are always valid, even for very small pores (example: carbon nanotubes with diameter under 1 nm). Nevertheless, some phenomena appear when the surface/volume ratio increases as it is the case in a small-size pore. Capillarity or non-zero velocity condition at walls are some examples but won't be addressed in this lecture. For gas, it is much more complicated as the porous media can affect the mean free path, i.e. the mean distance covered by a gas molecule before hitting another one. Let us compute the mean free path of a gas molecule.

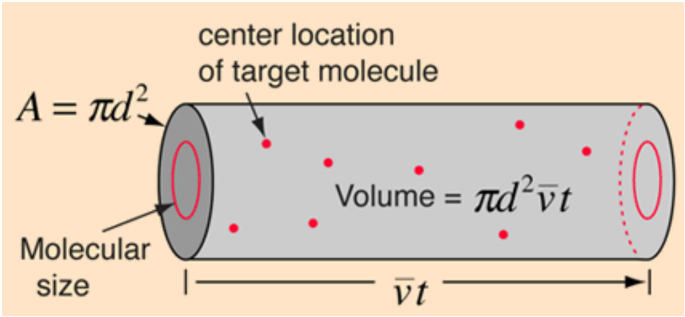


Figure 1.1: Volume crossed by a particle before collision with another one.

A particle (spherical, diameter d) can hit an other particle if its center is located at less than one diameter from the center of another particle. The Serway's point of view considers that a particle, travelling at an average velocity $\bar{v}$, has a specific surface of πd^2. It corresponds to the section of an equivalent particle needed to hit ponctual particles during its travel. We thus consider that other particles are points. During a time t, the effective particle (diameter $2d$) travels across a volume:

$$V = \pi d^2 \bar{v} t. \tag{1.1}$$

The mean free path can be estimated as the ratio between the path length and the number of other particles in the volume:

$$\lambda = \frac{\bar{v} t}{\pi d^2 \bar{v} t n_V}, \tag{1.2}$$

where n_V is the number of particles per unit volume. Actually this description does not take into account that other particles are moving too. We have to consider the average relative velocity $\bar{v_r} = \bar{v_1} - \bar{v_2}$. We can write:

$$\bar{v_r}^2 = \bar{v_1}^2 + \bar{v_2}^2 - 2\bar{v_1}\bar{v_2}. \tag{1.3}$$

As the velocities of each particles are statistically uncorrelated and random ($\bar{v_1}\bar{v_2} = 0$) and the average particle velocity is uniform on the particle population ($\bar{v_1} = \bar{v_2} = \bar{v}$), we have:

$$\bar{v_r} = \sqrt{2}\bar{v}. \tag{1.4}$$

In the mean free path expression given above, we have to replace the velocity $\bar{v}$ by $\bar{v_r}$ only in the denominator as this term corresponds to the interactions between the particles. Moreover, the number of particles per volume unit can be estimated using the matter quantity n, the Avogadro number $\mathcal{N}_A$ and the ideal gas equation $PV = nRT$ (with classical notations):

$$n_V = \frac{n\mathcal{N}_A}{V} = \frac{\mathcal{N}_A P}{RT}, \tag{1.5}$$

and finally we have the mean free path:

$$\lambda = \frac{RT}{\sqrt{2}\pi d^2 \mathcal{N}_A P} \tag{1.6}$$

The molecular diameter of N_2 is about 0.32 nm. The mean free path under atmospheric pressure and ambient temperature is thus $\lambda = 9.2 \times 10^{-8}$ m

To have $Kn < 1$, we must have $d_{pore} > \lambda$. This corresponds to $d_{pore} > 9.2 \times 10^{-8}$ m= 92 nm. It corresponds to the limit macro-pores/meso-pores.

1.3 Main properties of a porous media

We define here some quantities necessary to describe the properties of a porous media.

1.3.1 Phases

A porous media is first described by its phases. Generally, σ is attributed to the solid phase. α, β and γ are related to fluid phases. A quantity related to phase β is noted Ψ_β (see Slides).

1.3.2 Pore size

The pore size ℓ_b (or sometimes noted ℓ_α) can be defined as the diameter of the largest circle or sphere included in the pore (depending on the dimension 2D or 3D). Generally the pore size distribution is skewned. Different measurement methods are available to obtain this distribution: image analysis (2D), RX tomography (3D), mercury or gas porosimetry (3D). We will discuss porosimetry later on.

1.3.3 Porosity and specific surface

The porosity is defined as the ratio between the α-phase volume over the total porous media volume (in the case of coexistence of only two phases):

$$\varepsilon = \frac{V_\alpha}{V_\alpha + V_\sigma}. \tag{1.7}$$

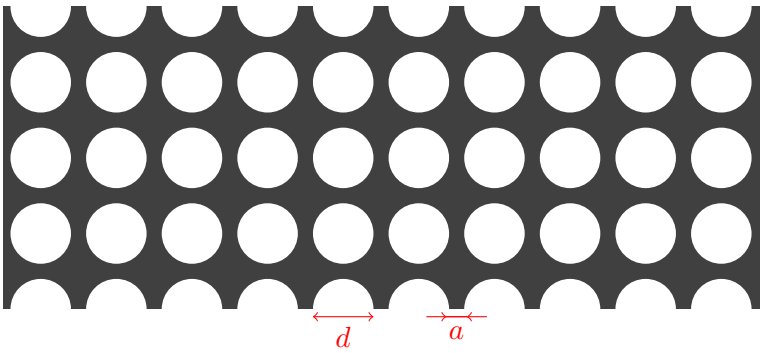
We will sometimes write ε_α to denote the porosity relative to the α phase. For a 3D arrangement of spherical particles, the lower porosity is reached for a hexagonal lattice where spheres are at contact.

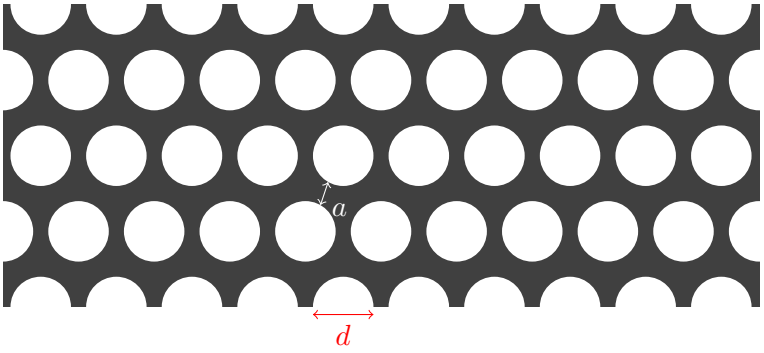
The specific surface corresponds to the surface of the solid phase divided bt the porous media volume. It is an important quantity as it will affect the transport in a porous media: the viscous energy loss is

related to the amount of surface-induced friction inside the porous media; the efficiency of a reactive porous media will directly depend on this specific surface. It can be write as:

$$S_S = \frac{S_\alpha}{V_\alpha + V_\sigma}. \tag{1.8}$$

We propose some examples of 2D and 3D periodic porous media. Pores (α-phase) are in white.

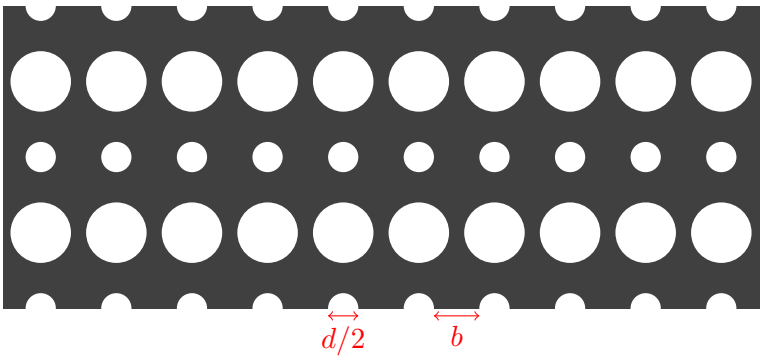




In the first configuration, the elementary "volume" is a square whose corners correspond to the center of four pores. The total surface is $(d+a)^2$ and the total pore surface is $\pi d^2/4$. The porosity is $\varepsilon = \pi/(4(1+a/d)^2)$.

The maximal porosity of the first configurations is reached when $a = 0$, the resulting porosity is $\varepsilon_{max} = \pi/4 \approx 0.79$.

For the second one, the elementary surface is an hexagon centered on a pore. There are three equivalent pores inside, and the total surface is $3\sqrt{3}(d+a)^2/2$. The porosity is finally $\varepsilon = \pi/\left(2\sqrt{3}(1+a/d)^2\right)$. The maximal porosity reaches, when $a = 0$, $\varepsilon_{max} = \pi/(2\sqrt{3}) \approx 0.91$.



For the third configuration, we take the same elementary surface as for the first configuration. Here, the total pore surface in the surface is $\pi d^2/8 + \pi d^2/32$. The total area is $(b + d/2)^2$. The resulting porosity reaches $\varepsilon = 5\pi/(32(1/2 + b/d)^2)$. The maximal porosity corresponds to contact between two large circles in the same row and between small and large circles in the same column. By doing the same development, as $b = d/2$, we get $\varepsilon_{max} = 5\pi/24 \approx 0.65$.

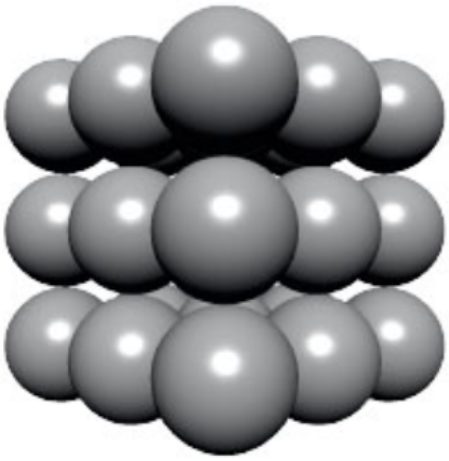


Figure 1.2: Side view

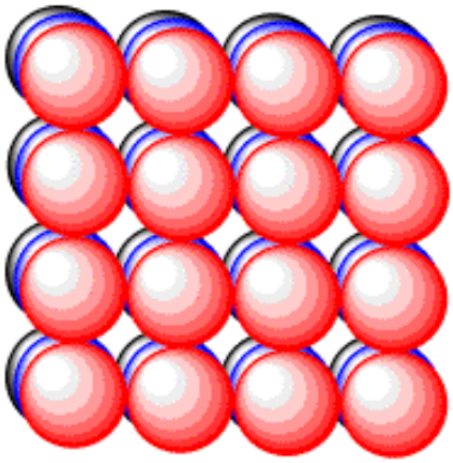


Figure 1.3: Top view

For the 3D configuration, the voids are not the sphere but the interstices between them. We have to consider a 3D elementary volume, which is actually a cube containing 4 quarters of sphere. The total solid volume in an elementary cube is $\pi d^3/6$ while the total volume is d^3. The resulting compactness is $C = \pi/6 \approx 0.52$ so the porosity is $\varepsilon = 1 - C = 1 - \pi/6 \approx 0.48$.

The specific surface is the ratio between the spheres surface in the volume (four quarters of sphere, πd^2) and the total volume (d^3) so $S_s = \pi/d$. The smaller is d, the larger is the specific surface. This is consistent with the fact that a reaction preformed using heterogeneous catalysis is generally more efficient with smaller particles.

Typically, a random packing of spherical particles has a porosity of about 0.4, whereas granite has a porosity of 0.01 (see Slides for more examples).

We want to draw an equivalence between porous media with different structures. By combining the expression of the porosity and of the specific surface is $S_v = \varepsilon \dfrac{S_\alpha}{V_\alpha} = (1 - \varepsilon)\dfrac{S_\alpha}{V_\sigma}$. For a porous media made of monodisperse spheres (radius a) we get :

$$S_v^{sph} = \frac{3(1 - \varepsilon)}{a}. \tag{1.9}$$

For an assembly of capillaries (radius R) we get:

$$S_v^{cyl} = \frac{2\varepsilon}{R}. \tag{1.10}$$

We fix ε and we want $S_v^{cyl} = S_v^{sph}$. It leads to an equivalent radius for the capillaries:

$$R_{eq} = \frac{2\varepsilon a}{3(1 - \varepsilon)} \tag{1.11}$$

1.3.4 Porosimetry

Porosity and pore size distribution can be measured using experimental methods. Mercury porosimetry uses the high surface tension of mercury (480 N/m at ambient temperature) to intrude it inside the porous media. Furthermore, the mercury generally does not wet solids.

Wettability is characterized by the contact angle of a liquid drop on a substrate. When a drop is on a surface, two other interfacial tensions (in addition to surface tension) will be involved: solid-air (γ_{SG}) and solid-liquid (γ_{SL}). See figure 1.4.

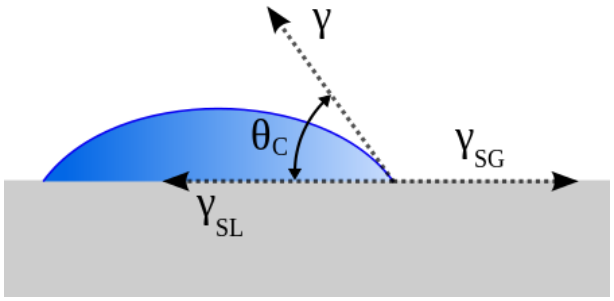


Figure 1.4: Sketch of the contact line forces in a drop.

We write the equilibrium of tensions along horizontal axis to obtain the contact angle (Young-Dupré law):

$$\gamma_{SG} = \gamma_{SL} + \gamma \cos\theta_c \Rightarrow \cos\theta_c = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma}. \tag{1.12}$$

The value of the contact angle gives a criterion for wettability of a surface. For mercury on classical solids, the contact angle is around 140°.

When a liquid is in a thin pore, due to surface tension, the liquid-gas interface is curved (meniscus), leading to a pressure drop through the interface (Laplace law):

$$P_L - P_G = -\frac{2\gamma\cos\theta_c}{R}, \tag{1.13}$$

where P_L and P_G are the pressure in the liquid and in the gas, respectively. R is the pore radius and γ the surface tension.

Given the numerical values and if we suppose that the porous media is in a vacuum chamber, we can write a semi-numerical version of the Washburn's law :

$$R = \frac{735\,\text{kPa}\cdot\text{m}}{P_L}. \tag{1.14}$$

For mercury porosimetry measurements, a sample is placed in a void chamber, and the chamber is filled of mercury. At zero pressure, the mercury cannot enter in the porous sample. By increasing the applied pressure P_L by controlled steps, a given volume of mercury will invade the sample at each step, which corresponds to a range of pore radii given by the previous formula. Finally, we can get the distribution of pore radius directly from this measurement.

Another technique is based on helium intrusion measurement. Two chambers are under vacuum, one is filled with the proous media. The void one is filled with helium. Then a valve is opened between the two chambers. The pressure variations give an insight about solid phase volume.

1.3.5 Tortuosity

The tortuosity is the ratio between the macroscopic size L of a porous media and the effective path L' to cross it. We denote $\tau = L'/L > 1$. It is a very basic definition which often needs refinements. For example, geometric and hydraulic path can differ due to fluid transport properties (see Slides).

1.3.6 Saturation

The saturation has two different definitions. In soil mechanics, the saturation w is the ratio between the mass of liquid over the mass of the solid matrix: $w = \frac{W_w}{W_s}$. In porous media physics, the saturation θ is defined as the ratio between the volume of liquid over the total volume of the porous media: $\theta = V_w/V$.

Lecture 2

Upscaling to porous media

Learning objectives At the end of this lecture, you should be able to:

- define the Representative Element Volume
- summarize the two different upscaling methods for porous media presented on the lecture
- explain the difference between intrinsic and superficial averages
- compute the spatial average of a scalar or a vector field in a porous media

2.1 First exampls : permeability of a composite porous media

We want to assess the permeability of a composite porous media. Figure 2.1 shows a porous media composed of N alternative layers whose thickness and permeability are respectively (h_1, k_1) and (h_2, k_2). The fluid has a viscosity η. A flow rate Q passes through the fully saturated porous media. Two configurations (a) and (b) (see figure 2.1) are considered. We assume that $L \gg h_1, h_2$.

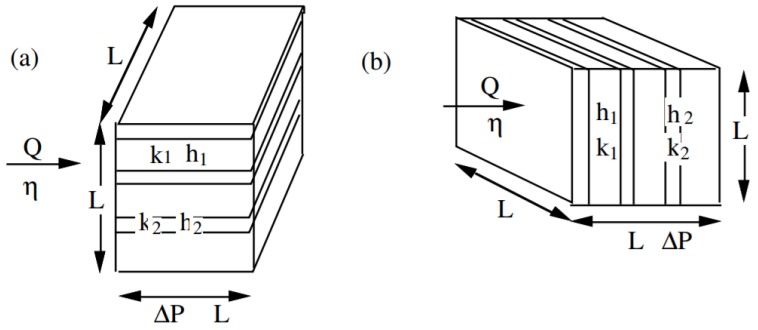


Figure 2.1: Composite porous media in two configurations relatively to the mass flux. Adapted from F. Moisy.

We start with the configuration (a). The flow rate is the sum of the flow rate through all the layers:

$$Q_{tot} = \frac{N}{2}Q_1 + \frac{N}{2}Q_2 = \frac{N}{2}\left(k_1 h_1 L\frac{\Delta P}{\eta L} + k_2 h_2 L\frac{\Delta P}{\eta L}\right). \tag{2.1}$$

The total section of the media is $A = L^2 = 0.5NL(h_1 + h_2)$. Consequently we can write the above expression as:

$$Q = k_{\parallel} A \frac{\Delta P}{\eta L}, \text{ with } k_{\parallel} = \frac{h_1 k_1 + h_2 k_2}{h_1 + h_2}. \tag{2.2}$$

For the second configuration, the flow rate must be conserved along the porous media. The flow rate through one layer $i = 1, 2$ is:

$$Q = Q_i = k_i L^2 \frac{\delta P_i}{\eta h_i}, \tag{2.3}$$

where δP_i is the pressure drop through the layer i considered. Actually we can write:

$$\Delta P = \frac{N}{2}(\delta P_1 + \delta P_2) \tag{2.4}$$

Consequently we can write:

$$Q_1 + \frac{h_2 k_1}{h_1 k_2} Q_2 = Q\left(1 + \frac{h_2 k_1}{h_1 k_2}\right) = k_1 L^2 \frac{\Delta P}{\eta h_1} \frac{2}{N}. \tag{2.5}$$

Since $2/N = (h_1 + h_2)/L$ (see above) and $A = L^2$, we get:

$$Q = k_{\perp} A \frac{\Delta P}{\eta L}, \text{ with } k_{\perp} = \frac{h_1 + h_2}{h_1/k_1 + h_2/k_2}. \tag{2.6}$$

If one of the $k_i \to 0$, $k_{\parallel} \to \dfrac{h_j k_j}{h_1 + h_2}$ with $j \neq i$, and $k_{\perp} \to 0$. If one of the $k_i \to \infty$, $k_{\parallel} \to \infty$, and $k_{\perp} \to \dfrac{h_1 + h_2}{h_j/k_j}$ with $j \neq i$.

Note that these two computations could be made using an electrical analogy. The permeability can be seen as the electrical conductivity.

2.2 Representative Elementary Volume

We consider a cylinder of sand grains (1 mm in diameter) as a model porous media. Its porosity is $\varepsilon = 0.36$. The number of pores in this system is of the same order of magnitude as the number of grains.

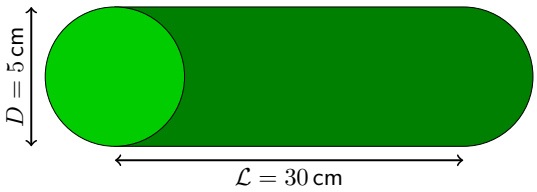


Figure 2.2: Example of core sample.

To know the number of sand grains, we must compute their total volume. The volume of the sample is $V = \pi D^2 \mathcal{L}/4 = 589\,\text{cm}^3$. The relation between porosity and sand volume is:

$$V_s = (1 - \varepsilon)V. \tag{2.7}$$

Thus $V_s = 377\,\text{cm}^3$. The volume of on sand grain is $v = \pi d^3/6 = 5.2 \times 10^{-4}\,\text{cm}^3$ with d the sand grains diameter. Consequently, in this sample we find about $V_s/v = 720 \times 10^3$ sand grains. Consequently, it is not possible to describe individually each pore. That's why we need an averaged description of the media.

It is necessary to reduce the number of degrees of freedom, to pass from heterogeneous to homogeneous scale. This will allow to compute effective properties with limit conditions at macro scale. **A porous media is homogeneous, relatively to a given physical process when the effective coefficients involved in transport equations are independent from the position.** (Quintard & Whitaker, 1993).

The representative elementary volume is a volume range were porous media properties are about constant while moving the volume around its position, or while slightly changing its typical size. A REV can be structural and/or relative to a physical process. The existence of this or these REV is necessary to compute homogeneization of the porous media, i.e. to get effective transport properties in the porous media.

2.3 Upscaling

If at least a structural REV exists (and sometimes a REV for the considered physical process), there are several methods to upscale the physical process from micro to macro scale, i.e. to access to the global properties from local (pore) properties.

2.3.1 Volume-averaging: theorems

The volume-averaging method aims at averaging over the REV the different physical quantities necessary to get a macroscopic description (laws, effective parameters, ...) of the local laws in the porous medium. It is mathematically based on theorems linking average of spatial variations (gradient, divergence, ...) to spatial variations of average of physical values. Similar theorems exist for temporal variations. Figure 2.3 shows the geometrical representation of the REV. A REV is placed at a position $\overrightarrow{x}$ and the relative position of any point in this REV is determined by $\overrightarrow{y_\alpha}$. $\overrightarrow{r_\alpha}$ represents the spatial position of any point in the porous media.

We can define two kinds of average for a quantity Ψ_α related to the phase α. Note that these averages are made **on the REV** so their values vary along the porous media. The average is made on $\overrightarrow{y_\alpha}$ and depends on $\overrightarrow{x}$. The **superficial average** is made over all the phases:

$$\langle \Psi_\alpha \rangle = \frac{1}{V} \int_{V_\alpha} \Psi_\alpha(\overrightarrow{x} + \overrightarrow{y_\alpha}) dV. \tag{2.8}$$

The **intrinsic average** is performed only on the concerned phase:

$$\langle \Psi_\alpha \rangle^\alpha = \frac{1}{V_\alpha} \int_{V_\alpha} \Psi_\alpha(\overrightarrow{x} + \overrightarrow{y_\alpha}) dV. \tag{2.9}$$

V represents the REV total volume and V_α represents the volume of the α-phase in the REV. We get directly $\langle \Psi_\alpha \rangle = \varepsilon_\alpha \langle \Psi_\alpha \rangle^\alpha$ with $\varepsilon_\alpha = V_\alpha/V$ the α-phase volume fraction.

Two main theorems are necessary for volume averaging. Their demonstration is out of the scope of this lecture. Concerning the gradient:

$$\langle \overrightarrow{\text{grad}} \Psi_\alpha \rangle = \overrightarrow{\text{grad}} \langle \Psi_\alpha \rangle + \frac{1}{V} \int_{S_{\alpha\sigma}} \Psi_\alpha \overrightarrow{n_{\alpha\sigma}} dS. \tag{2.10}$$

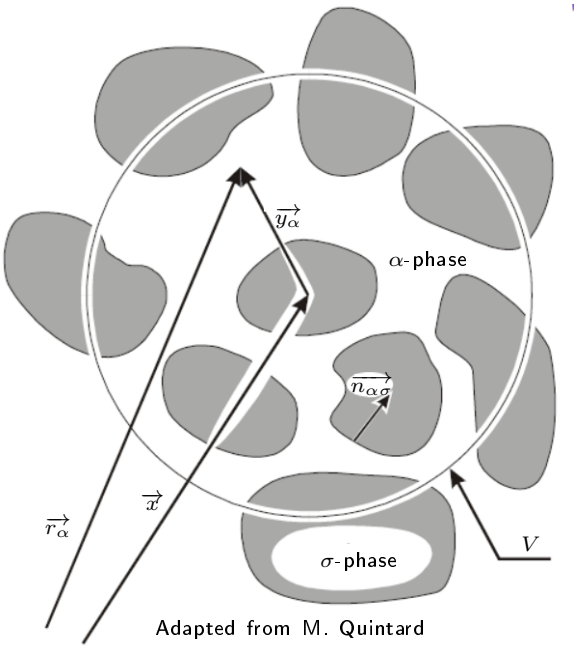


Figure 2.3: Sketch of the geometrical configuration of the REV.

Concerning the divergence:

$$\langle \mathrm{div}\overrightarrow{\Psi_\alpha}\rangle = \mathrm{div}\langle\overrightarrow{\Psi_\alpha}\rangle + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\Psi_\alpha}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{2.11}$$

$S_{\alpha\sigma}$ is the interface surface between phases α and σ in the considered REV. $\overrightarrow{n_{\alpha\sigma}}$ is the normal vector at $\alpha-\sigma$ interface (from α to σ phase). Note that these theorems concern here the superficial average.

$\frac{1}{V}\int_{S_{\alpha\sigma}} \Psi_\alpha\overrightarrow{n_{\alpha\sigma}}dS$ and $\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\Psi_\alpha}\cdot\overrightarrow{n_{\alpha\sigma}}dS$ are interfacial integrals. They are related to porous media structure (tortuosity, ...).

We can give some precisions about the interfacial integrals. We separate the physical quantity as $\Psi_\alpha = \langle\Psi_\alpha\rangle^\alpha + \widetilde{\Psi_\alpha}$. The interfacial term can be written as:

$$\frac{1}{V}\int_{S_{\alpha\sigma}} \Psi_\alpha\overrightarrow{n_{\alpha\sigma}}dS = \frac{1}{V}\int_{S_{\alpha\sigma}} \langle\Psi_\alpha\rangle^\alpha\overrightarrow{n_{\alpha\sigma}}dS + \frac{1}{V}\int_{S_{\alpha\sigma}} \widetilde{\Psi_\alpha}\overrightarrow{n_{\alpha\sigma}}dS. \tag{2.12}$$

The first term of the right hand of this equation, using scale separation and the fact that the average is computed on the whole REV, can be written:

$$I = \frac{1}{V}\int_{S_{\alpha\sigma}} \langle\Psi_\alpha\rangle^\alpha\overrightarrow{n_{\alpha\sigma}}dS = \langle\Psi_\alpha\rangle^\alpha\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{n_{\alpha\sigma}}dS, \tag{2.13}$$

since there typical length variation of $\langle\Psi_\alpha\rangle^\alpha$ is much larger than the REV length scale. To compute the integral term we use the averaging theorem for Ψ_α assuming for the computation an uniform (and non-zero) virtual field Ψ:

$$\langle\overrightarrow{\mathrm{grad}}\Psi\rangle = \overrightarrow{0} = \overrightarrow{\mathrm{grad}}\langle\Psi\rangle + \Psi\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{n_{\alpha\sigma}}dS. \tag{2.14}$$

With the relation $\langle\Psi\rangle = \varepsilon_\alpha \langle\Psi\rangle^\alpha$, we get[1]

$$-\frac{1}{\Psi}\left(\langle\Psi\rangle^\alpha \overrightarrow{\text{grad}}\varepsilon_\alpha + \varepsilon_\alpha \overrightarrow{\text{grad}}\langle\Psi\rangle^\alpha\right) = \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{n_{\alpha\sigma}} dS. \tag{2.15}$$

Using the definition of $\langle\Psi\rangle^\alpha$, we have:

$$\frac{\overrightarrow{\text{grad}}\varepsilon_\alpha}{\Psi V_\alpha}\int_{V_\alpha} \Psi dV + \frac{\varepsilon}{\Psi}\overrightarrow{\text{grad}}\left(\frac{1}{V_\alpha}\int_{V_\alpha}\Psi dV\right) = -\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{n_{\alpha\sigma}} dS. \tag{2.16}$$

Because Ψ is uniform, we finally get:

$$\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{n_{\alpha\sigma}} dS = -\overrightarrow{\text{grad}}\varepsilon_\alpha, \tag{2.17}$$

which does not depend on the virtual field Ψ. So, going back to Ψ_α, $I = -\langle\Psi_\alpha\rangle^\alpha \overrightarrow{\text{grad}}\varepsilon_\alpha$. Thus finally

$$\frac{1}{V}\int_{S_{\alpha\sigma}} \Psi_\alpha \overrightarrow{n_{\alpha\sigma}} dS = -\langle\Psi_\alpha\rangle^\alpha \overrightarrow{\text{grad}}\varepsilon_\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \widetilde{\Psi_\alpha}\overrightarrow{n_{\alpha\sigma}} dS. \tag{2.18}$$

2.3.2 Volume averaging procedure

We start from a local equation involving a physical quantity[2] Ψ which depends on the position in the porous media, external forcing(s) and porous media properties (fluid viscosity, porous structure, ...). We apply the average theorems to the local equation. With the decomposition $\Psi = \langle\Psi\rangle^\alpha + \widetilde{\Psi}$ we can separate local average and fluctuations. Note that fluctuations are more or less proportionnal to gradient of the average.

We can split the averaged local equation in two equations: one obtained from averaging the main equations on Ψ, the other one by subtracting the averaged equation to the local one. We have now two equations on $\langle\Psi\rangle^\alpha$ and $\widetilde{\Psi}$. As for turbulence (Reynolds-Averaged Navier-Stokes – RANS), we need a closure to solve the problem. There are indeed too much unknown quantities.

First we use the scale separation to reduce the equation on $\widetilde{\Psi}$. Generally, if the porous media is homogeneous, it is enough to have a linear relation between $\widetilde{\Psi}$ and $\langle\Psi\rangle^\alpha$. If not, we must use some heuristic relations. Finally, by injecting the linear relation into the averaged equation we get an equation between averaged quantity ($\langle\Psi\rangle^\alpha$, mean forcing(s)) involving effective properties of the porous media (for example its permeability).

2.3.3 Example: volume-averaging of the hydrostatics equation

To start using the volume-averaging method, we will apply it to a simple local equation: the hydrostatics equation:

$$-\overrightarrow{\text{grad}}P + \rho_\alpha \overrightarrow{g} = \overrightarrow{0}, \tag{2.19}$$

where P is the pressure of the fluid α-phase. The boundary condition is $P = P_0$ for $\overrightarrow{r_\alpha} = \overrightarrow{0}$ where $\overrightarrow{r_\alpha}$ locates points in the α-phase as illustrated in figure 2.4.

[1] Remind: $\overrightarrow{\text{grad}}(fg) = f\overrightarrow{\text{grad}}g + g\overrightarrow{\text{grad}}f$

[2] Here we suppress the $_\alpha$ index for better readability.

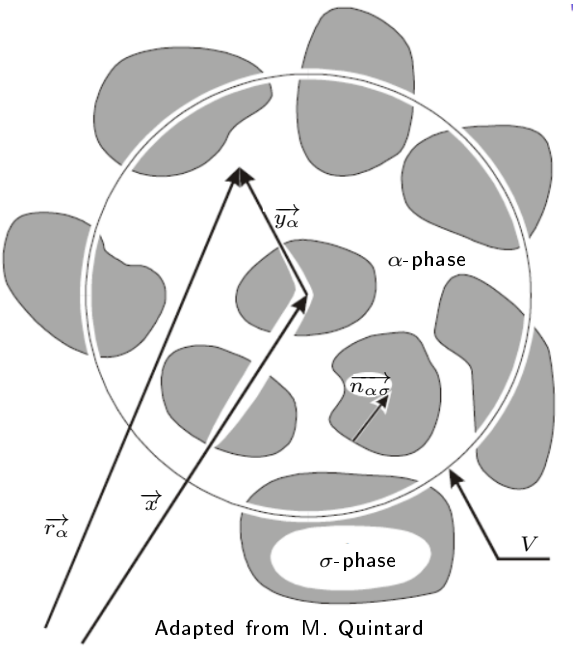


Figure 2.4: Sketch of the REV.

We remind the definition of the gradient: $dP = \overrightarrow{\text{grad}}P \cdot \overrightarrow{dr_\alpha}$. It leads to:

$$\overrightarrow{0} = \overrightarrow{\text{grad}}P \cdot \overrightarrow{dr_\alpha} + \rho\,\overrightarrow{g} \cdot \overrightarrow{dr_\alpha} = dP + \rho\,\overrightarrow{g} \cdot \overrightarrow{dr_\alpha}. \tag{2.20}$$

After integration, with the boundary condition, we have:

$$P = \rho\,\overrightarrow{g} \cdot \overrightarrow{r_\alpha} + P_0. \tag{2.21}$$

We remind that the definition of the intrinsic average for P is $\langle P\rangle^\alpha = \dfrac{1}{V_\alpha}\int_{V_\alpha} P(\overrightarrow{x} + \overrightarrow{y_\alpha})dV$. Using the intrinsic average we get (as $\overrightarrow{g}$ is uniform):

$$\langle P\rangle^\alpha = \rho\langle\overrightarrow{r_\alpha}\rangle^\alpha \cdot \overrightarrow{g} + P_0. \tag{2.22}$$

Using the geometrical decomposition of $\overrightarrow{r_\alpha}$, and reminding that the average is made on a REF of position $\overrightarrow{x}$, we get:

$$\langle P\rangle^\alpha = \rho\,\overrightarrow{x} \cdot \overrightarrow{g} + \rho\langle\overrightarrow{y_\alpha}\rangle^\alpha \cdot \overrightarrow{g} + P_0. \tag{2.23}$$

We apply the gradient operator to the previously obtained equation. By noticing that the gradient here represents the derivative with respect to $\overrightarrow{x}$ we have immediately:

$$\overrightarrow{\text{grad}}\langle P\rangle^\alpha = \rho\,\overrightarrow{g} + \rho\overrightarrow{\text{grad}}\langle\overrightarrow{y_\alpha}\rangle^\alpha \cdot \overrightarrow{g}. \tag{2.24}$$

The gradient of a vector is a tensor. The scalar product of a tensor and of a vector is a vector. Finally, the previous equation is a vectorial equation.

We note r_0 the typical scale of the REV, $\mathcal{L}$ the macroscale and ℓ_α the pore typical size. We make the assumption of scale separation: $\ell_\alpha \ll r_0 \ll \mathcal{L}$. As the gradient is with respect to $\overrightarrow{x}$, it is of

order of magnitude of $1/\mathcal{L}$. The typical variation of $\langle \overrightarrow{y_\alpha} \rangle^\alpha$ in the REV is of the order of magnitude r_0. Thus, $||\overrightarrow{\text{grad}} \langle \overrightarrow{y_\alpha} \rangle^\alpha|| \sim r_0/\mathcal{L} \ll 1$. Finally we get the volume-averaged hydrostatics equation in a porous media:

$$\overrightarrow{\text{grad}} \langle P \rangle^\alpha \approx \rho \overrightarrow{g}. \tag{2.25}$$

This equation is very similar to the local one, but it can be obtained only under scale separation assumption.

2.3.4 Asymptotic development

This method was proposed by Auriault and Sanchez-Palencia during the 80's and 90's.

We assume that we have for our porous media a REV with typical dimension r. The macroscopic dimension is called $\mathcal{L}$. Another hypothesis concerns the scale separation: $r \ll \mathcal{L}$.

We define the small element δ as:

$$\delta = \frac{r}{\mathcal{L}} \ll 1. \tag{2.26}$$

Note that the physical quantities must also check the scale separation conditions. That means that the local gradient of the quantity must be of the same order of magnitude as the gradient of the averaged quantity. For more precisions and an example, see Auriault (1991), p. 786.

We introduce two dimensionless space variables based on the physical space variable $\overrightarrow{X}$: $\overrightarrow{X}/r$ and $\overrightarrow{X}/\mathcal{L}$. Ψ is a physical field. It can be a state function (temperature for example) or a flux-based quantity (velocity for example). Under the assumption of scale separation, Ψ is a function of the two previous dimensionless space variables, among other variables. For conveniency we choose space physical variables $\overrightarrow{x}$ and $\overrightarrow{y} = \overrightarrow{x}/\delta$. $\overrightarrow{x}$ is the macroscopic (slow) variable and $\overrightarrow{y}$ is the microscopic (fast) one. Consequently we have:

$$\Psi(\overrightarrow{x}, \overrightarrow{y}) \text{ with } \overrightarrow{y} = \overrightarrow{x}/\delta, \tag{2.27}$$

which is the macroscopic point of view, or:

$$\Psi(\overrightarrow{x}, \overrightarrow{y}) \text{ with } \overrightarrow{x} = \delta \overrightarrow{y}, \tag{2.28}$$

which is the microscopic point of view.

We denote as $\langle \Psi \rangle$ the spatial average of Ψ. This average is taken on the REV. We have generally:

$$\Psi = \mathcal{O}(\langle \Psi \rangle), \tag{2.29}$$

where $\mathcal{O}(\,\cdot\,)$ must be understood compared to δ:

$$\Psi = \mathcal{O}(\langle \Psi \rangle) \text{ if } \delta \ll \frac{\Psi}{\langle \Psi \rangle} \ll \delta^{-1}. \tag{2.30}$$

The scale separation for Ψ can be translated as (see figure on the slides):

$$\frac{\partial \Psi}{\partial \overrightarrow{y}} = \mathcal{O}\left(\frac{\partial \langle \Psi \rangle}{\partial \overrightarrow{x}} \right) \Rightarrow \frac{\partial \Psi}{\partial \overrightarrow{y}} = \mathcal{O}\left(\frac{\partial \Psi}{\partial \overrightarrow{x}} \right). \tag{2.31}$$

It means that the local gradient of Ψ is of the same order of magnitude as the macroscopic gradient of $\langle\Psi\rangle$. See figure on the slides. The variation of $\langle\Psi\rangle$ against $\overrightarrow{x}$ over a length r is small (zero in the limit $\delta \to 0$). It means that Ψ is locally spatially stationary at micro-scale ($\overrightarrow{y}$-stationary). The average varis slowly at the microscopic scale. Ψ is stationary if its average is invariant through a local translation of order r.

Similarly to Taylor developments, using mathematical theorems, we can write an asymptotic development:

$$\Psi(\overrightarrow{x},\overrightarrow{y}) = \Psi^{(0)}(\overrightarrow{x},\overrightarrow{y}) + \delta\Psi^{(1)}(\overrightarrow{x},\overrightarrow{y}) + \delta^2\Psi^{(2)}(\overrightarrow{x},\overrightarrow{y}) + ..., \tag{2.32}$$

where $\Psi^{(i)}(\overrightarrow{x},\overrightarrow{y})$ are $\overrightarrow{y}$-stationary. Perfect homogenisation is reached for $\delta \to 0$. In this condition, $\Psi(\overrightarrow{x},\overrightarrow{y}) = \langle\Psi\rangle$.

Using this development, it is now possible to get a homogenized description of the local (microscopic) laws by replacing the physical quantities by their asymptotic forms. But it is beyond the scope of this lecture and we will preferably detail the following method.

Lecture 3

Hydrodynamic transport in porous media

Objectives At the end of this lecture, you should be able to:

- write and interpret the Darcy's law
- compute the Darcy's law using the volume-averaging method and a step-by-step guide
- compute an estimation of the permeability of a simple porous media
- perform the demonstration of the Kozeny-Carman relation
- define the Klinkenberg effect
- write the Darcy's law without neglecting inertia (Forccheimer's law)
- apply the Ergun's law to compute a permeability
- choose the good approach to assess the hydrodynamic transport in a porous media

3.1 Flow rate in a porous media

We make a first estimation of the flow rate of a fluid (viscosity η) in a porous media submitted to a pressure drop ΔP. Let us assume a system made of n identical cylinders (diameter D, length L). The cylinders are parallel and the porosity of this porous media is denoted as ε. The total porous media volume is V.

The mean fluid velocity in one cylinder is:

$$\bar{v} = \frac{D^2 \Delta P}{32 \eta L}. \tag{3.1}$$

Here the average could be assimilated to the intrinsic average. The flow rate through one cylinder is then:

$$q = \frac{\pi D^4 \Delta P}{128 \eta L}. \tag{3.2}$$

The total flow rate through the porous media is given by:

$$Q = US = nq, \tag{3.3}$$

where S is the total section of the porous media and U the **superficial** average velocity through the porous media. Thus,

$$U = \frac{n}{SL}\frac{\pi D^4 \Delta P}{128\eta}. \tag{3.4}$$

Furthermore, the porosity can be written as:

$$\varepsilon = \frac{n}{V} L\pi \frac{D^2}{4}. \tag{3.5}$$

The specific surface in this porous media is:

$$a = \frac{n\pi DL}{V}. \tag{3.6}$$

Finally we have, since $LS = V$:

$$U = \varepsilon \frac{D^2}{32}\frac{\Delta P}{\eta L} = \frac{\varepsilon^3}{2a^2}\frac{\Delta P}{\eta L}. \tag{3.7}$$

U is also called *filtration velocity*. In this formula we have a dependency only with macroscopic quantities (L), forcing (ΔP), fluid property (η) and porous media macroscopic characteristics (ε and a). It does not depend on the local porous structure. Consequently, this approach is a good approximation of the fluid average velocity through a porous media.

If the cylinders are tortuous, they have a length $L' = L\tau$. We must replace L by $L\tau$ in all the formula. Nevertheless, the volume V of the porous media remains equal to SL. Consequently we get:

$$U' = \frac{U}{\tau^2}. \tag{3.8}$$

3.2 Volume-averaging: application to Stokes flow in a porous media

The previous development is only a model and has a lack of generality. We will know get a macroscopic equation to know the relation between the fluid velocity through a porous media and an applied pressure drop.

We know the behaviour of a fluid flowing in one pore using Stokes equation. But the way it affects the global flow rate through the porous media is not trivial. Actually, we try to find the well-known Darcy's law using the volume-averaging method whose process is detailed in the previous chapter and in the Slides.

3.2.1 Microscopic equations

We assume a porous media saturated by one liquid (α-phase). The porous structure (σ-phase) is rigid and at rest in the operator's referential. We neglect gravity effects. A pressure drop is applied through the porous media. We assume scale separation, local equilibrium and existence of a REV for both structure and physical quantities. The local Stokes flow is driven by the equations:

$$\eta \Delta \overrightarrow{v} = \overrightarrow{\text{grad}} P, \tag{3.9}$$

$$\operatorname{div} \overrightarrow{v} = 0, \tag{3.10}$$

where P is the pressure, $\overrightarrow{v}$ the fluid velocity, η the fluid dynamic viscosity. We add the boundary conditions:

$$\overrightarrow{v} = \overrightarrow{0} \quad \text{at} \quad S_{\alpha\sigma} \tag{3.11}$$

$$\overrightarrow{v} = \overrightarrow{f}(\overrightarrow{r}, t) \quad \text{at} \quad S_{\alpha e}, \tag{3.12}$$

where $S_{\alpha\sigma}$ is the surface between solid and liquid phase, $S_{\alpha e}$ the surface between the liquid phase and entrance and exit from the porous media.

3.2.2 Continuity equation

Let us start with the continuity equation. The average of the velocity divergence is still zero. Thus, using the second theorem (see slides), we get:

$$\langle \operatorname{div} \overrightarrow{v} \rangle = \operatorname{div} \langle \overrightarrow{v} \rangle + \frac{1}{V} \int_{S_{\alpha\sigma}} \overrightarrow{v} \cdot \overrightarrow{n_{\alpha\sigma}} dS = 0, \tag{3.13}$$

where $\overrightarrow{n_{\alpha\sigma}}$ is the normal vector at the interface between liquid and solid phases. Since the fluid cannot inter-penetrate the solid phase ($\overrightarrow{v} \cdot \overrightarrow{n_{\alpha\sigma}} = 0$), the interfacial integral is zero, thus $\operatorname{div} \langle \overrightarrow{v} \rangle = 0$. We remind the relation between intrinsic and superficial average:

$$\langle \overrightarrow{v} \rangle = \varepsilon_\alpha \langle \overrightarrow{v} \rangle^\alpha, \tag{3.14}$$

thus the continuity equation can be written under the alternative form using the intrinsic average[1]:

$$\operatorname{div} \langle \overrightarrow{v} \rangle^\alpha = -\varepsilon_\alpha^{-1} \overrightarrow{\operatorname{grad}} \varepsilon_\alpha \cdot \langle \overrightarrow{v} \rangle^\alpha. \tag{3.15}$$

This is the first averaged equation of the problem.

3.2.3 Momentum equation

The superficial average of the Stokes equation is (neglecting the gravity):

$$\eta \langle \Delta \overrightarrow{v} \rangle = \langle \overrightarrow{\operatorname{grad}} P \rangle. \tag{3.16}$$

Concerning the pressure term, we get:

$$\langle \overrightarrow{\operatorname{grad}} P \rangle = \overrightarrow{\operatorname{grad}} \langle P \rangle + \frac{1}{V} \int_{S_\alpha} P \overrightarrow{n_{\alpha\sigma}} dS, \tag{3.17}$$

and finally[2], as $\langle P \rangle = \varepsilon_\alpha \langle P \rangle^\alpha$,

[1] Remember: $\operatorname{div}(f\vec{A}) = f \operatorname{div} \vec{A} + \overrightarrow{\operatorname{grad}} f \cdot \vec{A}$.

[2] Remember: $\overrightarrow{\operatorname{grad}}(fg) = f \overrightarrow{\operatorname{grad}} g + g \overrightarrow{\operatorname{grad}} f$.

$$\langle\overrightarrow{\text{grad}}P\rangle = \varepsilon_\alpha\overrightarrow{\text{grad}}\langle P\rangle^\alpha + \langle P\rangle^\alpha\overrightarrow{\text{grad}}\varepsilon_\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} P\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.18}$$

We need here to explicit the interfacial integral to get an equation for $\langle P\rangle^\alpha$. We apply the decomposition in average and fluctuations for the pressure:

$$P = \langle P\rangle^\alpha + \widetilde{P}. \tag{3.19}$$

Given the interfacial integral expressions (see Slides), we have:

$$\langle\overrightarrow{\text{grad}}P\rangle = \varepsilon_\alpha\overrightarrow{\text{grad}}\langle P\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \widetilde{P}\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.20}$$

Let us observe the viscous term. We can write the Laplacian operator as the divergence of the gradient of $\overrightarrow{v}$. The gradient of a vector is a tensor. Divergence of a tensor results in a vector. We have:

$$\langle\Delta\overrightarrow{v}\rangle = \langle\text{div}(\overrightarrow{\text{grad}}\overrightarrow{v})\rangle = \text{div}(\langle\overrightarrow{\text{grad}}\overrightarrow{v}\rangle) + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\overrightarrow{v}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.21}$$

Using the decomposition $\overrightarrow{v} = \langle\overrightarrow{v}\rangle^\alpha + \widetilde{\overrightarrow{v}}$, we get:

$$\langle\Delta\overrightarrow{v}\rangle = \text{div}(\langle\overrightarrow{\text{grad}}\overrightarrow{v}\rangle) + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\langle\overrightarrow{v}\rangle^\alpha\cdot\overrightarrow{n_{\alpha\sigma}}dS + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.22}$$

The averaged velocity variation over a REV is negligible (scale separation) so its gradient can be taken out of the integral. We recover the integral computed at eq. 2.17 and finally we get:

$$\langle\Delta\overrightarrow{v}\rangle = \text{div}(\langle\overrightarrow{\text{grad}}\overrightarrow{v}\rangle) - \overrightarrow{\text{grad}}\varepsilon_\alpha\cdot\overrightarrow{\text{grad}}\langle\overrightarrow{v}\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.23}$$

We apply again the averaging theorem to the velocity gradient under the divergence:

$$\langle\Delta\overrightarrow{v}\rangle = \Delta\langle\overrightarrow{v}\rangle + \text{div}\left(\frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{v}\overrightarrow{n_{\alpha\sigma}}dS\right) - \overrightarrow{\text{grad}}\varepsilon_\alpha\cdot\overrightarrow{\text{grad}}\langle\overrightarrow{v}\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.24}$$

Using the no-slip boundary condition, we can remove the term under the divergence so:

$$\langle\Delta v\rangle = \Delta\langle\overrightarrow{v}\rangle - \overrightarrow{\text{grad}}\varepsilon_\alpha\cdot\overrightarrow{\text{grad}}\langle\overrightarrow{v}\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS. \tag{3.25}$$

Finally, for the momentum equation we have the volume-averaged version:

$$\varepsilon_\alpha\overrightarrow{\text{grad}}\langle P\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \widetilde{P}\overrightarrow{n_{\alpha\sigma}}dS = \eta\left(\Delta\langle\overrightarrow{v}\rangle - \overrightarrow{\text{grad}}\varepsilon_\alpha\cdot\overrightarrow{\text{grad}}\langle\overrightarrow{v}\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS\right). \tag{3.26}$$

This is the second averaged equations we need.

We assume a constant porosity thus terms involving porosity spatial variations can be discarded. Moreover, using the relation $\langle\overrightarrow{v}\rangle = \varepsilon_\alpha\langle\overrightarrow{v}\rangle^\alpha$, we have[3]

[3]Remember: $\Delta(fg) = f\Delta g + g\Delta F + 2\overrightarrow{\text{grad}}f\overrightarrow{\text{grad}}g$.

$$\varepsilon_\alpha \overrightarrow{\text{grad}}\langle P\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \widetilde{P}\overrightarrow{n_{\alpha\sigma}}dS = \eta\left(\varepsilon_\alpha \Delta\langle\overrightarrow{v}\rangle^\alpha + \frac{1}{V}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS\right) \tag{3.27}$$

3.2.4 Equations on fluctuations

We need now to close the equation relatively to the velocity. We remind that the local continuity equation writes as $\text{div}\,\overrightarrow{v} = 0$ and that we have the decomposition $\overrightarrow{v} = \langle\overrightarrow{v}\rangle^\alpha + \widetilde{\overrightarrow{v}}$. Thus, the continuity equation 3.15 can be written as:

$$\text{div}\,\widetilde{\overrightarrow{v}} = \varepsilon_\alpha^{-1}\overrightarrow{\text{grad}}\varepsilon_\alpha \cdot \langle\overrightarrow{v}\rangle^\alpha. \tag{3.28}$$

Once again, we assume an homogeneous porous media where porosity is constant (actually the porosity typical variation length is much larger than the intrinsic velocity). Consequently,

$$\text{div}\,\widetilde{\overrightarrow{v}} = 0. \tag{3.29}$$

This is the first equation for fluctuations.

Concerning the momentum equation, we can subtract equation 3.27 to equation 3.9, leading to (after dividing by ε_α):

$$\overrightarrow{\text{grad}}\widetilde{P} - \frac{1}{V_\alpha}\int_{S_{\alpha\sigma}} \widetilde{P}\overrightarrow{n_{\alpha\sigma}}dS = \eta\left(\Delta\widetilde{\overrightarrow{v}} - \frac{1}{V_\alpha}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS\right). \tag{3.30}$$

This is the second equation for fluctuations.

3.2.5 Closure

We need now to close the system. We can notice that the fluctuations $\widetilde{\overrightarrow{v}}$ and $\widetilde{P}$ solve a smilar equation system with boundary conditions as $\overrightarrow{v}$ and P (eqs 3.9-3.12):

$$\begin{aligned}
\text{div}\,\widetilde{\overrightarrow{v}} &= 0, && (3.31)\\
\overrightarrow{\text{grad}}\widetilde{P} - \frac{1}{V_\alpha}\int_{S_{\alpha\sigma}} \widetilde{P}\overrightarrow{n_{\alpha\sigma}}dS &= \eta\left(\Delta\widetilde{\overrightarrow{v}} - \frac{1}{V_\alpha}\int_{S_{\alpha\sigma}} \overrightarrow{\text{grad}}\widetilde{\overrightarrow{v}}\cdot\overrightarrow{n_{\alpha\sigma}}dS\right), && (3.32)\\
\widetilde{\overrightarrow{v}} &= \langle\overrightarrow{v}\rangle^\alpha \quad \text{at} \quad S_{\alpha\sigma}, && (3.33)\\
\widetilde{\overrightarrow{v}} &= \overrightarrow{g}(\overrightarrow{r},t) \quad \text{at} \quad S_{\alpha e}, && (3.34)\\
\langle\widetilde{\overrightarrow{v}}\rangle^\alpha &= \overrightarrow{0}. && (3.35)
\end{aligned}$$

An additional constraint (the last equation) is necessary. Furthermore, note that $\langle\overrightarrow{v}\rangle^\alpha$ and $\overrightarrow{g}(\overrightarrow{r},t)$ are source terms for the velocity.

As the intrinsic velocity acts as a constant source, we choose it to propose a solution for the spatial fluctuations velocity and pressure. We can now assume that the velocity and pressure fluctuations have the following form:

$$\begin{aligned}
\widetilde{\overrightarrow{v}} &= \overline{\overline{B}}\cdot\langle\overrightarrow{v}\rangle^\alpha && (3.36)\\
\widetilde{P} &= \eta\,\overrightarrow{b}\cdot\langle\overrightarrow{v}\rangle^\alpha. && (3.37)
\end{aligned}$$

The tensor $\overline{\overline{B}}$ and the vector $\overrightarrow{b}$ depend only on geometric considerations of the porous media. Equation 3.35 shows indeed that the velocity spatial fluctuations depend on a constant source term on the REV.

Since on the integration domain $S_{\alpha\sigma}$ the intrinsic average of the velocity is constant, we can write from equation 3.27

$$\overrightarrow{\text{grad}}\langle P\rangle^\alpha = \eta\Delta\langle\overrightarrow{v}\rangle^\alpha - \eta\varepsilon_\alpha\overline{\overline{K}}^{-1}\langle\overrightarrow{v}\rangle^\alpha, \tag{3.38}$$

where

$$\frac{1}{V_\alpha}\int_{S_{\alpha\sigma}}\overrightarrow{\text{grad}}\overline{\overline{B}}\cdot\overrightarrow{n_{\alpha\sigma}}dS - \frac{1}{V_\alpha}\int_{S_{\alpha\sigma}}\overrightarrow{b}\cdot\overrightarrow{n_{\alpha\sigma}}dS = -\varepsilon_\alpha\overline{\overline{K}}^{-1}. \tag{3.39}$$

$\overline{\overline{K}}$ is the **permeability tensor**. For an isotropic media, it is scalar and constant. We finally have:

$$\langle\overrightarrow{v}\rangle = -\frac{\overline{\overline{K}}}{\eta}\overrightarrow{\text{grad}}\langle P\rangle^\alpha + \overline{\overline{K}}\cdot\Delta\langle\overrightarrow{v}\rangle^\alpha. \tag{3.40}$$

This is known as the Darcy's law, with the Brinkman correction (last term). We can estimate some orders of magnitude to see if it is possible to discard this correction. We have $\overline{\overline{K}}\sim\ell_\alpha^2$ where ℓ_α is the typical pore size. Consequently $\overline{\overline{K}}\cdot\Delta\langle\overrightarrow{v}\rangle^\alpha\sim\frac{\ell_\alpha^2}{L_v^2}\langle\overrightarrow{v}\rangle$, where L_v is the typical dimension of variation of the average velocity. This dimension is much larger then the REV typical dimension which is larger than ℓ_α. Consequently we can neglect the Brinkman correction, in homogeneous porous media when there is not extreme velocity gradient in the volume averaged. We finally have:

$$\langle\overrightarrow{v}\rangle = -\frac{\overline{\overline{K}}}{\eta}\overrightarrow{\text{grad}}\langle P\rangle^\alpha. \tag{3.41}$$

$\langle P\rangle^\alpha$ is the classical pressure we use in hydrodynamics. $\langle\overrightarrow{v}\rangle$ is called the Darcy's velocity (or filtration velocity). It can be related to the flow rate as:

$$Q = KA\frac{\Delta P}{\eta L} \tag{3.42}$$

for an isotropic media. A and L are the macroscopic section and length of the studied porous media.

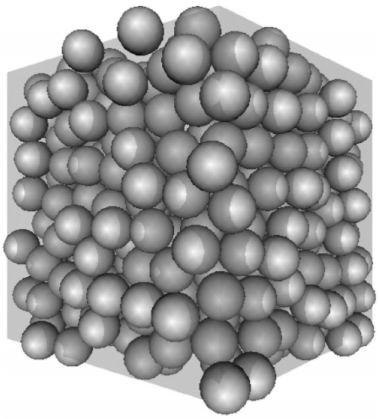
We must now estimate the value of the permeability tensor for different kind of porous media (Hele-Shaw cell, sand grains assembly, ...).

3.3 Kozeny-Carman relation for porous media permeability

In a Hele Shaw cell, we have a Poiseuille flow between two planes. We denote as L the length and b as its thickness ($b\ll L$); the width of cell is considered large compared to these two lengths. We apply a pressure drop ΔP, the fluid mean velocity is:

$$\bar{v} = \frac{b^2\Delta P}{12\eta L}. \tag{3.43}$$

Given the Darcy law, we have a permeability $K = b^2/12$.



We consider now a packing of n spheric particles with porosity ε and volume V. The porosity expression is:

$$\varepsilon = \frac{V_{pores}}{V_{tot}} = 1 - \frac{V_{particles}}{V_{tot}} = 1 - \frac{n\pi}{6}\frac{D^3}{V}. \tag{3.44}$$

The specific surface is:

$$a = \frac{S_{particles}}{V} = \frac{n\pi D^2}{V}. \tag{3.45}$$

Consequently we get:

$$\varepsilon = 1 - \frac{aD}{6} \Leftrightarrow a = (1-\varepsilon)\frac{6}{D}. \tag{3.46}$$

We have seen earlier that the average velocity of fluid flowing through an assembly of tortuous parallel cylinders can be written as:

$$U = \frac{\varepsilon^3}{2\tau^2 a^2}\frac{\Delta P}{\eta L}, \tag{3.47}$$

where τ is the tortuosity. We can consider it as a model case of porous media. We apply it to the grains assembly and in this case, using the Darcy's law and the relation between the specific surface and the porosity, the permeability is:

$$k = \frac{\varepsilon^3 D^2}{72\tau^2(1-\varepsilon)^2}. \tag{3.48}$$

To estimate the tortuosity, we can consider a fluid flowing around a sphere. If it is in contact with this sphere, its path length is $L' = \pi D/2$, whereas the "macroscopic" length of the sphere is $L = D$. Consequently, the torutosity is $\tau = L'/L = \pi/2$. We finally get:

$$k = \frac{\varepsilon^3 D^2}{18\pi^2(1-\varepsilon)^2} \approx \frac{\varepsilon^3 D^2}{180(1-\varepsilon)^2}. \tag{3.49}$$

It is named Kozeny-Carman relation. The prefactor 1/180 depends on the real spatial organisation of the beads, the size polydispersity, the particle deformation, ...

3.4 Corrections to the Darcy's law

The Darcy's law is not always valid in the form presented above. Some phenomena, such as inertia or a large Knudsen number, can affect its expression.

3.4.1 Apparent permeability with inertia

If the flow through the porous media is inertial, the apparent permeability will be lower than the expected one from Darcy's law. This is due to appearance of recirculation cells inside the porous media leading to a reduction of the effective section of the pores. If the Reynolds number at pore scale is larger than 1–10, inertia must be taken into account.

Using homogeneization technique(s) we get the Darcy-Forchheimer's law:

$$\overrightarrow{\text{grad}}\langle P\rangle^\alpha = -\eta\overline{\overline{K}}^{-1}\langle\overrightarrow{v}\rangle - \rho\beta\langle\overrightarrow{v}\rangle^2. \tag{3.50}$$

β is independent of the fluid, it depends only on the porous media. Locally we can write $\overrightarrow{\text{grad}}P = -\overline{\overline{K}}^{-1}\overrightarrow{v} - \rho\beta||\overrightarrow{v}||\overrightarrow{v}$.

By a factorization of $\eta\overline{\overline{K}}^{-1}$ we get an apparent permeability:

$$\langle\overrightarrow{v}\rangle = -\frac{\overline{\overline{K}}_{app}}{\eta}\overrightarrow{\text{grad}}\langle P\rangle^\alpha \text{ with } K_{app} = \frac{\overline{\overline{K}}}{1+\varepsilon\beta\sqrt{\overline{\overline{K}}}Re_p^*}, \tag{3.51}$$

and $Re_p^* = \dfrac{\rho\sqrt{\overline{\overline{K}}}||\langle\overrightarrow{v}\rangle||}{\eta\varepsilon}$. This Reynolds number is based on the pore velocity ($||\langle\overrightarrow{v}\rangle||/\varepsilon$) and a length scale built on the square root of the permeability.

3.4.2 Ergun's law

We derive the Ergun relation which is the relation analogous to the Kozeny-Carman one for inertial flows. The system is similar as for the previous Kozeny-Carman relation: the porous media is considered as an assembly of tortuous cylinder with the same porosity and specific surface as the real porous media. We consider an assembly of n cylinders (length L, diameter D) with an applied pressure difference ΔP and a fluid of viscosity η. The real porous media is a particle assembly (diameter D_p) whose porosity and specific surface are equal to the cylinder assembly. The pressure drop in the case of a laminar flow can be written (Poiseuille's law):

$$\frac{\Delta P}{L} = \frac{32\eta L\bar{v}}{D^2}, \tag{3.52}$$

with $\bar{v}$ the mean fluid velocity in one cylinder (similar to the intrinsic average). We have seen (Kozeny-Carman relation) that for a laminar flow through a bed of particles of diameter D with porosity ε,

$$\frac{\Delta P}{L} = 180\frac{(1-\varepsilon)^2}{\varepsilon^3}\frac{\eta U}{D_p^2}, \tag{3.53}$$

where U is the mean velocity through the porous media and D_p the particle diameter.

We add an inertial contribution for energy dissipation. For the part corresponding to the inertial contribution, we can make a dimensional analysis. The pressure difference ΔP has the dimension of

a volume energy. It must be proportional to the kinetic energy per volume $0.5\rho\bar{v}^2$. Moreover, the pressure difference is classically proportional to the pipe length L. To keep the good dimension we must divide by D which is constant along the pipe. Finally we have:

$$\frac{\Delta P}{L} = \frac{\rho}{2\,D}\bar{v}^2 \tag{3.54}$$

for the inertial contribution. Let us remind that $U = \varepsilon\bar{v}$ for the whole porous media. Moreover, for a cylinder assembly, we have:

$$\varepsilon = \frac{n}{V}L\pi\frac{D^2}{4} \text{ and } a = \frac{n\pi DL}{V} \text{ so } \varepsilon = a\frac{D}{4}. \tag{3.55}$$

For a particle bed we have:

$$\varepsilon = 1 - \frac{aD_p}{6}. \tag{3.56}$$

Using these relations to remove D and replace it by D_p, and because we fixed ε and a we have:

$$\frac{\Delta P}{L} = \frac{\rho a}{8\varepsilon^3}U^2 \;\Rightarrow\; \frac{\Delta P}{L} = \frac{3\rho(1-\varepsilon)}{4\,D_p\varepsilon^3}U^2. \tag{3.57}$$

The energy loss of the flow in the porous media is the addition of the viscous contribution and the inertial one. Since the pressure drop must depend on the tortuosity and that kinetic energy dissipation should depend on the number of particles by unit of length, Ergun added a correction coefficient β:

$$\frac{\Delta P}{L} = \frac{180(1-\varepsilon)^2}{\varepsilon^3}\frac{\eta}{D_p^2}U + \beta\frac{3\,(1-\varepsilon)}{4\,\varepsilon^3}\frac{\rho}{D_p}U^2. \tag{3.58}$$

Ergun (1951) and Macdonald (1979) respectively showed experimentally that $3\beta/4 = 1.75$ and $3\beta/4 = 1.8$ for smooth particles. For rough particles, $3\beta/4 = 4.0$

3.4.3 Gas flow through a porous media: Klinkenberg effect

This section is an auto-learning exercise (see Moodle). It consists in analysing an article with questions as a guideline in order to understand the Klinkenberg effect and its consequences on gas flow through a porous media. The following computations refer to some developments proposed during the exercise.

The objective here is to analytically compute the pressure profile through the porous media. The permeability for a gas is a function of the pressure, according to Klinkenberg (1941):

$$k_g = k_\infty\left(1 + \frac{b}{P}\right), \tag{3.59}$$

where k_∞ is the premeability for infinite pressure, P the pressure and b the Klinkenberg factor. The Darcy's law neglecting the gravity term is (replacing the average notations by standard notations):

$$\overrightarrow{v} = -\frac{k_g}{\eta}\overrightarrow{\text{grad}P}, \tag{3.60}$$

with standard notations for the viscosity. The ideal gas relation is $\rho = \beta P$ with $\beta = M_g/RT$) with ρ the gas density and M_g the molar mass of the gas. Finally the mass conservation for a gas writes as (with porosity ε):

$$\mathrm{div}(\rho\overrightarrow{v}) + \varepsilon\frac{\partial\rho}{\partial t}. \tag{3.61}$$

By combining ideal gas relation, Darcy's law, mass conservation and Klinkenberg permeability, we get:

$$\varepsilon\beta\frac{\partial P}{\partial t} = \mathrm{div}\left(\frac{k_\infty\beta}{\eta}(P+b)\overrightarrow{\mathrm{grad}}P\right). \tag{3.62}$$

We define $P_b = P + b$. The previous equation can be re-written as:

$$\frac{1}{\alpha}\frac{\partial P_b^2}{\partial t} = \mathrm{div}(\overrightarrow{\mathrm{grad}}P_b^2), \tag{3.63}$$

with $\alpha = \dfrac{k_\infty P_b}{\varepsilon\eta}$. This is valid for a scalar permeability (homogeneous and isotropic problem).

If we consider a 1D, stationary problem, we can simplify the eq. 3.62:

$$\frac{\partial}{\partial x}\left(\frac{k_\infty\beta}{\eta}(P+b)\frac{\partial P}{\partial x}\right) = 0. \tag{3.64}$$

The integration of the previous equation (using the definition of P_b) gives:

$$P_b^2 = \frac{2\eta}{k_\infty\beta}Ax + B, \tag{3.65}$$

where A and B are integration constants. We have two boundary conditions. First, $P_b(L) = P_L$, then we have a fix flow rate at porous media entrance: $q_m = \rho(x=0)v(x=0)$. With the Darcy's law we can write:

$$q_m = \beta P(x=0)\left(-\frac{k_\infty}{\eta}\right)\left(1 + \frac{b}{P(x=0)}\right)\frac{\partial P}{\partial x}|_{x=0}, \tag{3.66}$$

which can be reduced as:

$$q_m = -\frac{\beta k_\infty}{2\eta}\frac{\partial P_b^2}{\partial x}|_{x=0}, \tag{3.67}$$

which finally gives $A = -q_m$. The use of the first boundary condition results in $B = P_L^2 + \dfrac{2\eta q_m}{k_\infty\beta}L$ and finally the pressure profile is:

$$P = -b + \sqrt{b^2 + P_L^2 + 2bP_L + \frac{2q_m\eta}{k_\infty\beta}(L-x)} \tag{3.68}$$

If we now consider an axi-symmetric configuration and stationarity, we can write eq. 3.62 as:

$$\mathrm{div}(\overline{\overline{k_\infty}}P_b\overrightarrow{\mathrm{grad}}P_b) = \mathrm{div}\left(k_{r,\infty}P_b\frac{\partial P_b}{\partial r}\overrightarrow{e_r} + k_{z,\infty}P_b\frac{\partial P_b}{\partial z}\overrightarrow{e_z}\right). \tag{3.69}$$

To do that we consider a permeability tensor $\overline{\overline{k_\infty}}$ with three diagonal components. As $P_b\partial P_b = \frac{1}{2}\partial P_b^2$ we finally get:

$$k_{r,\infty}\frac{\partial^2 P_b^2}{\partial r^2} + k_{r,\infty}\frac{1}{r}\frac{\partial P_b^2}{\partial r} + k_{z,\infty}\frac{\partial^2 P_b^2}{\partial z^2} = 0. \tag{3.70}$$

Lecture 4

Dispersion and diffusion in porous media

Mass transport in porous media is fundamental in numerous industrial applications such as filtration systems. Several mechanisms can affect dispersion and diffusion of particles inside the porous media: advection by a fluid, molecular diffusion, mechanical dispersion due to porous structure, interactions between a solute and the porous matrix. We will detail these different phenomena in order to understand the main mechanisms and parameters at play in dispersion and diffusion of particles/molecules in porous media.

Objectives At the end of this lecture, you should be able to:

- write and apply the Fick's law
- name the different kind of dispersion mechanisms in a porous media
- demonstrate the Taylor's dispersion in a pipe
- describe diffusion phenomenon in porous media
- write and interpret the advection-dispersion equation including the diffusion tensor
- adapt the Taylor's dispersion to natural media

4.1 Dispersion in a homogeneous media

When particles are present in a fluid, thermal agitation makes them move from high to low concentrations. A phenomenological law (Fick's law) gives:

$$\overrightarrow{q} = -D_m \overrightarrow{\text{grad}}\phi, \tag{4.1}$$

where $\overrightarrow{q}$ is the flux density vector, D_m is the molecular diffusivity coefficient ans ϕ an intensive physical quantity (such as concentration).

The diffusivity can be affected by walls (very present in porous media) which leads to anisotropic diffusion. The scalar molecular diffusivity can become a tensor.

When particles are advected and diffuse, we can derive the **advection-diffusion equation**.

We will derive the advection-dispersion equation in its general form. Let us consider a physical intensive quantity (concentration, temperature, ...) held by a fluid. Two mechanisms can locally affect

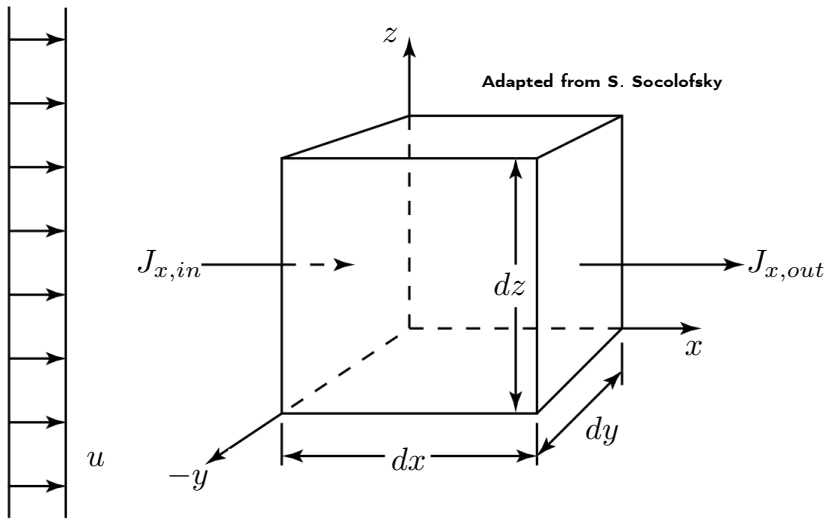


Figure 4.1: Sketch of a control volume with crossflow.

this quantity $C(x, y, z, t)$: molecular/particle diffusion and convection/advection due to the flow. We consider a control volume as the one presented figure 4.1. Advection and diffusion are supposed to be linearly independent. The total flux of particles entering in the control volume in the x direction can be written as:

$$J_{x,in} = \frac{1}{dt}(u(x, y, z, t)C(x, y, z, t)dzdydt + q_x dzdydt), \tag{4.2}$$

where q_x is the flux density vector due to diffusion and u the advection velocity. Let us remind the Fick's law:

$$\overrightarrow{q} = -D_m \overrightarrow{\text{grad}} C. \tag{4.3}$$

Consequently we get:

$$J_{x,in} = u(x, y, z, t)C(x, y, z, t)dydz - D_m \frac{\partial C}{\partial x}|_x dydz \tag{4.4}$$

and

$$J_{x,out} = u(x + dx, y, z, t)C(x + dx, y, z, t)dydz - D_m \frac{\partial C}{\partial x}|_{x+dx} dydz. \tag{4.5}$$

Finally the total flux in the x direction through the volume control is:

$$J_x = J_{x,in} - J_{x,out} = -\frac{\partial(uC)}{\partial x}dxdydz + \frac{\partial}{\partial x}\left(D_m \frac{\partial C}{\partial x}\right)dxdydz. \tag{4.6}$$

If we generalize at three dimensions, assuming a global velocity $\overrightarrow{v} = (u, v, w)$, we have:

$$J = (-\text{div}(\overrightarrow{v}C) + \text{div}(D_m \overrightarrow{\text{grad}} C))dxdydz. \tag{4.7}$$

Using the conservation principle (mass conservation, energy conservation, ...) we can write that the total flux through the control volume is equal to the inner time-variation of the physical quantity integrated in this volume:

$$\frac{\partial C dxdydz}{\partial t} = (\mathrm{div}(D_m \overrightarrow{\mathrm{grad}} C) - \mathrm{div}(\overrightarrow{v} C))dxdydz \tag{4.8}$$

so finally

$$\frac{\partial C}{\partial t} = \mathrm{div}(D_m \overrightarrow{\mathrm{grad}} C) - \mathrm{div}(\overrightarrow{v} C), \tag{4.9}$$

which is the general form of the advection-diffusion equation. The first term of the right hand corresponds to molecular diffusion whereas the second term concerns the flow convection.

If we consider an uniform diffusivity and incompressible flow, we get a simplified form[1]:

$$\frac{\partial C}{\partial t} = D_m \Delta C - \overrightarrow{v} \cdot \overrightarrow{\mathrm{grad}} C. \tag{4.10}$$

4.2 Dispersion in porous media

4.2.1 Volume-averaged advection-diffusion equation

The different methods developed in the previous chapter can be applied to the local advection-diffusion equation. The detailed computation is beyond the scope of this chapter but can be a good exercise for the reader. With the same notations as previously established, we get for the intrinsic average of the solute concentration:

$$\varepsilon \frac{\partial \langle C \rangle^\alpha}{\partial t} = \varepsilon \mathrm{div}\left(\overline{\overline{D}} \cdot \overrightarrow{\mathrm{grad}} \langle C \rangle^\alpha\right) - \mathrm{div}(\langle \overrightarrow{v} \rangle \langle C \rangle^\alpha). \tag{4.11}$$

$\overline{\overline{D}}$ is the effective diffusion (or dispersion) tensor. The main question now is to get some insights about the different mechanisms of dispersion in a porous media.

4.2.2 Dispersion mechanisms

If we consider no flow through the porous media, only molecular diffusion can provoke dispersion of a solute in the porous media. For the same macroscopic distance travelled by a self-diffusion molecule in a porous media or in a homogeneous media, the particle in a porous media must travel a higher absolute distance due to tortuosity τ. Molecular diffusion is thus hindered. We can write an effective molecular diffusion coefficient as:

$$D_m^{eff} = \frac{D_m}{\tau} \quad (\tau > 1). \tag{4.12}$$

When a fluid transports some particles in a porous media, there is a a superimposition of convection due to fluid and diffusion, especially in dead-end pores. Furthermore, in a pore, the heterogeneities of velocity (Poiseuille-like flows) lead to a dispersion of the transported species. Finally, due to porous structure, streamlines can be separated leading to high dispersion of the particles. We will detail some of these mechanisms.

[1] Remember: $\mathrm{div}(f\overrightarrow{g}) = f\mathrm{div}\,\overrightarrow{g} + \overrightarrow{g} \cdot \overrightarrow{\mathrm{grad}} f$

4.2.3 Taylor-Aris dispersion

This mechanism of dispersion is due to velocity inhomogeneities in the porous media, especially in the pore section (Poiseuille-like flow). Added to molecular diffusion, this is a very efficient mixing way.

We consider a non-uniform advection velocity in a pipe. Especially, the gradients perpendicularly to the flow will be sharper than in the case of only molecular diffusion. In a straight cylindrical pipe, we have $\overrightarrow{v} = v(r)\overrightarrow{e_z}$ in the cylindrical coordinates (r, θ, z) with:

$$v(r) = 2\bar{v}\left(1 - \frac{r^2}{a^2}\right) \text{ with } \bar{v} = \frac{1}{\pi a^2}\int_0^{2\pi}\int_0^a v(r) r dr d\theta = \frac{2}{a^2}\int_0^a v(r) r dr. \tag{4.13}$$

a is the pipe radius and $\bar{v}$ is the average velocity over the pipe's cross-section. Using the same definition for the cross-section average, we denote as $\bar{x}$ the average quantity of x over the pipe. Be careful: $\overline{xy} \neq \bar{x}\bar{y}$.

We assume an axi-symmetric distribution of the physical quantity $C(r, z, t)$ at $t = 0$. Using the advection-dispersion equation for incompressible flow and uniform diffusivity, we shall write:

$$\frac{\partial C}{\partial t} + v(r)\frac{\partial C}{\partial z} = D_m \Delta C = D_m\left(\frac{\partial^2 C}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C}{\partial r}\right)\right). \tag{4.14}$$

Since the boundary is not permeable, we have $\frac{\partial C}{\partial r}|_{r=a} = 0$.

We separate C into a cross-section average and a r-dependent part:

$$C(r, z, t) = \bar{C}(z, t) + C'(r, z, t) \text{ with } \bar{C} = \frac{2}{a^2}\int_0^a C r dr. \tag{4.15}$$

From equation 4.14 we get:

$$\frac{\partial \bar{C}}{\partial t} + \frac{\partial C'}{\partial t} + v(r)\frac{\partial \bar{C}}{\partial z} + v(r)\frac{\partial C'}{\partial z} = D_m\left(\frac{\partial^2 \bar{C}}{\partial z^2} + \frac{\partial^2 C'}{\partial z^2} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C'}{\partial r}\right)\right) \tag{4.16}$$

Note that $\overline{C'} = 0$ and $\overline{\bar{C}} = \bar{C}$. Temporal derivative and average can be switched. Taking the cross-section average of equation 4.16 we write:

$$\frac{\partial \bar{C}}{\partial t} + \overline{v(r)}\frac{\partial \bar{C}}{\partial z} + \overline{v(r)\frac{\partial C'}{\partial z}} = D_m \frac{\partial^2 \bar{C}}{\partial z^2}. \tag{4.17}$$

As $\bar{C}$ does not depend on r, it is constant for the average operator and can ben factorized. After computation of the average, the last term of equation 4.16 has been removed using $\frac{\partial C}{\partial r}|_{r=a} = 0$. The transport of $\bar{C}$ thus depends on the average advection of the r-dependant part of C. The aim here is to obtain an advection-dispersion equation on $\bar{C}$ with an effective diffusivity. To do that we need to compute the expression of C' to get an equation invomving only $\bar{C}$.

Substracting 4.17 from 4.16 we get:

$$\frac{\partial C'}{\partial t} + (v(r) - \bar{v})\frac{\partial \bar{C}}{\partial z} + v(r)\frac{\partial C'}{\partial z} - \overline{v(r)\frac{\partial C'}{\partial z}} = D_m \Delta C'. \tag{4.18}$$

To be able to solve this equation we need some assumptions. We can observe write that after a time of order of a^2/D_m the cross-pipe molecular diffusion have almost smoothed out variation of C

in the radial direction. It means that for $t \sim t^* = \mathcal{O}(a^2/D_m)$, $\bar{C} \gg C'$. For particles with radius $R = 100\,\text{nm}$ in water at ambient temperature we get $D_m \approx 10^{-12}\,\text{m}^2/\text{s}$, using the Stokes-Einstein relation. Consequently we have $t^* \approx 1\,\text{s}$ for a pore of radius $1\,\mu\text{m}$. We consider know that we work at $t \ll t^*$ so the temporal variation of C' can be discarded and $\bar{C} \gg C'$.

Moreover we expect that gradients in the radial direction are greater than in the longitudinal direction. Consequently we can simplify the previous equation as:

$$(v(r) - \bar{v})\frac{\partial \bar{C}}{\partial z} \approx \frac{D_m}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C'}{\partial r}\right). \tag{4.19}$$

Using the expression of $v(r)$ we get:

$$\frac{\partial}{\partial r}\left(r\frac{\partial C'}{\partial r}\right) = \frac{1}{D_m}\bar{v}\frac{\partial \bar{C}}{\partial z}\left(r - \frac{2r^3}{a^2}\right). \tag{4.20}$$

Since $\bar{C}$ does not depend on r we can easily integrate twice this equation:

$$C' = \frac{1}{D_m}\bar{v}\frac{\partial \bar{C}}{\partial z}\left(\frac{r^2}{4} - \frac{r^4}{8a^2} + A + B\ln r\right). \tag{4.21}$$

Since C' cannot diverge at $r = 0$, we have $B = 0$. Moreover $\bar{C'} = 0$, which fixes $A = -\dfrac{a^2}{12}$. Finally we get:

$$C'(r,z) = \frac{a^2}{24D_m}\bar{v}\frac{\partial \bar{C}}{\partial z}\left(6\frac{r^2}{a^2} - 3\frac{r^4}{a^4} - 2\right). \tag{4.22}$$

Since we have an expression of C' we can compute the third term of equation 4.17:

$$\begin{aligned}
\overline{v(r)\frac{\partial C'}{\partial z}} &= \frac{\bar{v}^2}{6D_m}\frac{\partial^2 \bar{C}}{\partial z^2}\int_0^a \left(1 - \frac{r^2}{a^2}\right)\left(6\frac{r^2}{a^2} - 3\frac{r^4}{a^4} - 2\right) r\,dr & (4.23)\\
&= \frac{\bar{v}^2}{6D_m}\frac{\partial^2 \bar{C}}{\partial z^2}\int_0^a \left(-2r + 8\frac{r^3}{a^2} - 9\frac{r^5}{a^4} + 3\frac{r^7}{a^6}\right) dr & (4.24)\\
&= -\frac{a^2\bar{v}^2}{48D_m}\frac{\partial^2 \bar{C}}{\partial z^2}. & (4.25)
\end{aligned}$$

Using this relation in equation 4.17 we get a advection-dispersion equation on $\bar{C}$:

$$\frac{\partial \bar{C}}{\partial t} + \bar{v}\frac{\partial \bar{C}}{\partial z} = \left(D_m + \frac{a^2\bar{v}^2}{48D_m}\right)\frac{\partial^2 \bar{C}}{\partial z^2} = D_{eff}\frac{\partial^2 \bar{C}}{\partial z^2}. \tag{4.26}$$

D_{eff} is the effective downstream diffusion coefficient. It can be written as:

$$D_{eff} = D_m + \frac{a^2\bar{v}^2}{48D_m} = D_m\left(1 + \frac{Pe^2}{48}\right) \text{ with } Pe = \frac{a\bar{v}}{D_m}. \tag{4.27}$$

Pe is named the **Péclet number** and compares advection and diffusion phenomena.

To summarize, after the time $t^* = a^2/D_m$, the concentration is about uniform across the pipe and the material will have moved a distance $\bar{v}t$. It will have spread out of $\mathcal{O}(\sqrt{D_{eff}t})$ in the z direction.

4.2.4 Mechanical dispersion

Due to porous micro-structure, dispersion of particles flowing through a porous media is enhanced compared to a homogeneous media. It adds to Taylor dispersion and to (hindered) molecular diffusion. It will lead to separation of particles groups. Furthermore, It is a Fick-like dispersion with a diffusion tensor:

$$\overline{\overline{D}} = \begin{pmatrix} D_{k_\parallel} + D_m^{eff} & 0 & 0 \\ 0 & D_{k_\perp} + D_m^{eff} & 0 \\ 0 & 0 & D_{k_\perp} + D_m^{eff} \end{pmatrix} \tag{4.28}$$

$$\text{with } \begin{cases} D_{k_\parallel} = \alpha_\parallel ||\langle \overrightarrow{v} \rangle|| \\ D_{k_\perp} = \alpha_\perp ||\langle \overrightarrow{v} \rangle|| \end{cases} \quad \text{Scheidegger(1951)} \tag{4.29}$$

D_m^{eff} is the molecular diffusivity corrected by tortuosity, $D_m^{eff} = D_m/\tau$. α is the dispersivity which is based on geometrical structure of the porous media. For non-connected cylinder assembly, we get $\alpha_\perp = \alpha_\parallel = \dfrac{a^2 ||\langle \overrightarrow{v} \rangle||}{48 D_m}$ as there is only Taylor-Aris dispersion (in addition to molecular diffusion).

4.2.5 Influence of sorption on the porous matrix

Some porous media can have reactive solid surfaces. Because of adsorption and chemisorption of transported solutes, a source term must be added to the advection-dispersion equation. We have an additive source term:

$$Q_s(C) = -K \frac{\partial C}{\partial t}. \tag{4.30}$$

K is the characteristic sorption constant. We can define a delay factor: $R = 1 + K$. We remind that the Darcy velocity can be written as $\langle \overrightarrow{v} \rangle = \varepsilon \langle \overrightarrow{v} \rangle^\alpha$. Moreover the intrinsic average for the concentration is defined as $\langle C \rangle^\alpha = \dfrac{1}{V_\alpha} \int_{V_\alpha} C dV$.

Using volume averaging method, we get the advection-diffusion equation (with sorption) in a porous media :

$$R\varepsilon \frac{\partial \langle C \rangle^\alpha}{\partial t} = \varepsilon \text{div}(\overline{\overline{D}} \cdot \overrightarrow{\text{grad}} \langle C \rangle^\alpha) - \text{div}(\langle \overrightarrow{v} \rangle \langle C \rangle^\alpha), \tag{4.31}$$

where $\overline{\overline{D}}$ is the diffusion coefficient taking into account the previously detailed diffusion/dispersion mechanisms.

4.3 Example of 2-D dispersion in a porous media

We study here a situation where tracers are dispersing in a 2D porous media.

Given the advection-diffusion equation:

$$R\varepsilon \frac{\partial \langle C \rangle^\alpha}{\partial t} = \varepsilon \text{div}(\overline{\overline{D}} \cdot \overrightarrow{\text{grad}} \langle C \rangle^\alpha) - \text{div}(\langle \overrightarrow{v} \rangle \langle C \rangle^\alpha) \text{ with } R = 1 + K, \tag{4.32}$$

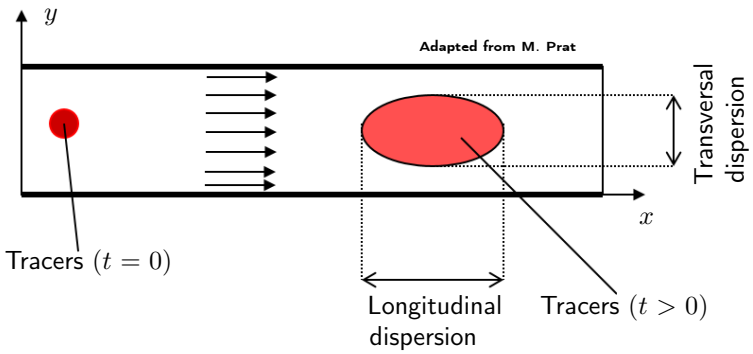


Figure 4.2: Flow and tracers in a porous media.

we can derive the specific equation verified by $\langle C\rangle^\alpha$. We consider no sorption so $R = 1$ and homogeneous porous media. But due to the flow, the dispersion is not isotropic. The flow can be considered as incompressible. We get quite easily by developping the last term and discarding the $\langle C\rangle^\alpha \mathrm{div}\langle\overrightarrow{v}\rangle$ term:

$$\varepsilon\frac{\partial\langle C\rangle^\alpha}{\partial t} = \varepsilon D_{\|}\frac{\partial^2\langle C\rangle^\alpha}{\partial x^2} + \varepsilon D_{\perp}\frac{\partial^2\langle C\rangle^\alpha}{\partial y^2} - \langle\overrightarrow{v}\rangle_x\frac{\partial\langle C\rangle^\alpha}{\partial x}, \tag{4.33}$$

with $D_{\|}$ and $D_{\perp}$ the longitudinal and transverse components of the diffusivity tensor.

The Péclet number can be written, using the Darcy velocity $\langle\overrightarrow{v}\rangle_x$:

$$Pe = \frac{\ell_\alpha\langle\overrightarrow{v}\rangle_x}{\varepsilon D_m} \tag{4.34}$$

with ℓ_α the typical pore dimension and D_m the molecular diffusivity.

4.4 Conclusion and applications

There is a main parameter which drives dispersion and diffusion in a porous media: **the Péclet number**. At low Péclet number, we can consider only the molecular diffusion (corrected by the tortuosity). Then we will observe superposition of molecular diffusion and mechanical dispersion, with a transition towards mechanical dispersion only. If the Péclet number is increased again, inertia effects will appear.

A typical example of application is the pollution of an aquifer: how the pollutants wil be transported and will spread inside the aquifer?

Lecture 5

Thermal transfer in porous media

Three main mechanisms allow to transfer heat: convection (with fluid moves), conduction (without matter move) and radiation. Each of these transport mechanisms are related to specific properties leading to specific transfer at interfaces.

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

- cite and describe the three thermal transfer mechanisms in porous media
- summarize the one-equation volume-averaged thermal conduction model
- interpret different models of equivalent conductivity
- differentiate natural and forced convection
- summarize the convection thermal transfer model
- define the Rayleigh and Nusselt numbers in porous media

5.1 Derivation of heat equation

We consider a media at rest where the thermal transfer is made only by conduction. We remind the Fourier's law:

$$\overrightarrow{\phi} = -\overline{\overline{\lambda}} \cdot \overrightarrow{\text{grad}T}, \tag{5.1}$$

with $\overrightarrow{\phi}$ the heat flux density vector, $\overline{\overline{\lambda}}$ the thermal conductivity tensor and T the temperature.

The first principle of the thermodynamic can be written, without source and considering no work:

$$\Delta U = Q. \tag{5.2}$$

Moreover we have $\Delta U = mc_v \Delta T$ which gives $Q = mc_v \Delta T$.

Now, we consider an elementary volume whose dimensions are (dx, dy, dz). The balance during time dt of internal energy in this volume can be given by:

$$dU = \phi_x(x,y,z)dydzdt - \phi_x(x+dx,y,z)dydzdt + \phi_y(x,y,z)dxdzdt - \phi_y(x,y+dy,z)dxdzdt \\ +\phi_z(x,y,z)dydxdt - \phi_z(x,y,z+dz)dydxdt. \tag{5.3}$$

Using a Taylor development, simplifying by dt and using the relation between U and T, we get:

$$mc_v\frac{\partial T}{\partial t} = -\mathrm{div}(\overrightarrow{\phi})dxdydz. \tag{5.4}$$

Since $m = \rho dxdydz$ where ρ is the density of the media, and using the Fourier's law, we finally get the heat equation for conduction:

$$\rho c_v\frac{\partial T}{\partial t} = \mathrm{div}(\overline{\overline{\lambda}}\cdot\overrightarrow{\mathrm{grad}T}). \tag{5.5}$$

5.2 Homogenization of the heat equation

Here we will detail the volume-averaged method to get the macroscopic law for thermal conduction in a porous media. The local equations and boundary conditions for the conduction problem in porous media are (for the fluid α-phase and the solid σ-phase):

$$(\rho c_v)_\sigma\frac{\partial T_\sigma}{\partial t} = \mathrm{div}(\overline{\overline{\lambda_\sigma}}\cdot\overrightarrow{\mathrm{grad}T_\sigma}), \tag{5.6}$$

$$(\rho c_v)_\alpha\frac{\partial T_\alpha}{\partial t} = \mathrm{div}(\overline{\overline{\lambda_\alpha}}\cdot\overrightarrow{\mathrm{grad}T_\alpha}), \tag{5.7}$$

$$T_\sigma = T_\alpha \text{ at } S_{\sigma\alpha}, \tag{5.8}$$

$$\overline{\overline{\lambda_\sigma}}\cdot\overrightarrow{\mathrm{grad}T_\sigma}\cdot\overrightarrow{n_{\alpha\sigma}} = \overline{\overline{\lambda_\alpha}}\cdot\overrightarrow{\mathrm{grad}T_\alpha}\cdot\overrightarrow{n_{\alpha\sigma}}. \tag{5.9}$$

We consider only one fluid phase and one solid phase. Using the volume averaging theorems (on the REV) and the definition of the intrinsic average (see slides), we get from equation 5.6 (solid phase):

$$(1-\varepsilon)(\rho c_v)_\sigma\frac{\partial\langle T_\sigma\rangle^\sigma}{\partial t} = \mathrm{div}\left[(1-\varepsilon)\overline{\overline{\lambda_\sigma}}\cdot\overrightarrow{\mathrm{grad}}\langle T_\sigma\rangle^\sigma + \frac{\overline{\overline{\lambda_\sigma}}}{V}\cdot\int_{S_{\sigma\alpha}} T_\sigma\overrightarrow{n}_{\sigma\alpha}dS\right] \\ +\frac{1}{V}\int_{S_{\sigma\alpha}}\overline{\overline{\lambda_\sigma}}\cdot\overrightarrow{n}_{\sigma\alpha}\cdot\overrightarrow{\mathrm{grad}}T_\sigma dS, \tag{5.10}$$

where ε is the porosity (homogeneous media). For the fluid phase we get similarly:

$$\varepsilon(\rho c_v)_\alpha\frac{\partial\langle T_\alpha\rangle^\alpha}{\partial t} = \mathrm{div}\left[\varepsilon\overline{\overline{\lambda_\alpha}}\cdot\overrightarrow{\mathrm{grad}}\langle T_\alpha\rangle^\alpha + \frac{\overline{\overline{\lambda_\alpha}}}{V}\cdot\int_{S_{\alpha\sigma}} T_\alpha\overrightarrow{n}_{\alpha\sigma}dS\right] \\ +\frac{1}{V}\int_{S_{\alpha\sigma}}\overline{\overline{\lambda_\alpha}}\cdot\overrightarrow{n}_{\alpha\sigma}\cdot\overrightarrow{\mathrm{grad}}T_\alpha dS, \tag{5.11}$$

Note that for these two volume-averaged equations, we do not have the same orientation of the $\alpha-\sigma$ interface's normal vector. For the σ-phase we have $\overrightarrow{n_{\sigma\alpha}}$ and for the α-phase we have $\overrightarrow{n_{\alpha\sigma}} = -\overrightarrow{n_{\sigma\alpha}}$.

We remind that the temperatures can be split in an average and a spatial fluctuations part: $T_\sigma = \langle T_\sigma \rangle^\sigma + \widetilde{T_\sigma}$ and $T_\alpha = \langle T_\alpha \rangle^\alpha + \widetilde{T_\alpha}$. Under order of magnitude arguments and other assumptions, it can be shown that (Carbonell and Whitaker, 1984):

$$\frac{1}{V_\sigma} \cdot \int_{S_{\sigma\alpha}} T_\sigma \overrightarrow{n}_{\sigma\alpha} dS \approx \frac{1}{V_\sigma} \cdot \int_{S_{\sigma\alpha}} \widetilde{T_\sigma} \overrightarrow{n}_{\sigma\alpha} dS, \tag{5.12}$$

and

$$\frac{1}{V_\alpha} \cdot \int_{S_{\alpha\alpha}} T_\alpha \overrightarrow{n_{\alpha\sigma}} dS \approx \frac{1}{V_\alpha} \cdot \int_{S_{\alpha\alpha}} \widetilde{T_\alpha} \overrightarrow{n_{\alpha\sigma}} dS. \tag{5.13}$$

The volume-averaged for the solid and fluid phases become respectively:

$$\begin{aligned}(1-\varepsilon)(\rho c_v)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = \operatorname{div} \left[(1-\varepsilon) \overline{\overline{\lambda_\sigma}} \cdot \overrightarrow{\operatorname{grad}} \langle T_\sigma \rangle^\sigma + \frac{\overline{\overline{\lambda_\sigma}}}{V} \cdot \int_{S_{\sigma\alpha}} \widetilde{T_\sigma} \overrightarrow{n}_{\sigma\alpha} dS \right] \\ + \frac{1}{V} \int_{S_{\sigma\alpha}} \overline{\overline{\lambda_\sigma}} \cdot \overrightarrow{n}_{\sigma\alpha} \cdot \overrightarrow{\operatorname{grad}} T_\sigma dS\end{aligned} \tag{5.14}$$

and

$$\begin{aligned}\varepsilon(\rho c_v)_\alpha \frac{\partial \langle T_\alpha \rangle^\alpha}{\partial t} = \operatorname{div} \left[\varepsilon \overline{\overline{\lambda_\alpha}} \cdot \overrightarrow{\operatorname{grad}} \langle T_\alpha \rangle^\alpha + \frac{\overline{\overline{\lambda_\alpha}}}{V} \cdot \int_{S_{\alpha\sigma}} \widetilde{T_\alpha} \overrightarrow{n}_{\alpha\sigma} dS \right] \\ + \frac{1}{V} \int_{S_{\alpha\alpha}} \overline{\overline{\lambda_\alpha}} \cdot \overrightarrow{n}_{\alpha\sigma} \cdot \overrightarrow{\operatorname{grad}} T_\alpha dS.\end{aligned} \tag{5.15}$$

The first integral of equations 5.14 and 5.15 corresponds to conductive exchanges between phases and the second one to porous structure effects. If we assume a local thermal equilibrium we can write:

$$\langle T_\sigma \rangle^\sigma = \langle T_\alpha \rangle^\alpha = T. \tag{5.16}$$

The validity of such an assumption is based on the comparison of characteristic times of thermal equilibrium at macroscopic scale and pore scale which leads to $(\ell_\alpha / \mathcal{L})^2 \ll 1$. It needs also a same order of magnitude of the thermal conductivities. By adding equation 5.15 to equation 5.14 and having in mind the boundary conditions and $\overrightarrow{n_{\sigma\alpha}} = -\overrightarrow{n_{\alpha\sigma}}$ we get the classical one-equation model:

$$(\rho c_v)^* \frac{\partial T}{\partial t} = \operatorname{div} \left[(\varepsilon \overline{\overline{\lambda_\alpha}} + (1-\varepsilon) \overline{\overline{\lambda_\sigma}}) \cdot \overrightarrow{\operatorname{grad}} T + \frac{1}{V} \cdot \int_{S_{\alpha\sigma}} (\overline{\overline{\lambda_\alpha}} \widetilde{T_\alpha} - \overline{\overline{\lambda_\sigma}} \widetilde{T_\sigma}) \cdot \overrightarrow{n}_{\alpha\sigma} dS \right] \tag{5.17}$$

with $(\rho c_v)^* = \varepsilon(\rho c_v)_\alpha + (1-\varepsilon)(\rho c_v)_\sigma$ the effective calorific capacity. Using the boundary conditions we see that on $S_{\sigma\alpha}$, $\widetilde{T_\alpha} = \widetilde{T_\sigma}$. Thus we get:

$$(\rho c_v)^* \frac{\partial T}{\partial t} = \operatorname{div} \left[(\varepsilon \overline{\overline{\lambda_\alpha}} + (1-\varepsilon) \overline{\overline{\lambda_\sigma}}) \cdot \overrightarrow{\operatorname{grad}} T + \frac{\overline{\overline{\lambda_\alpha}} - \overline{\overline{\lambda_\sigma}}}{V} \cdot \int_{S_{\alpha\sigma}} \widetilde{T_\alpha} \overrightarrow{n}_{\alpha\sigma} dS \right] \tag{5.18}$$

We close the problem assuming that the temperature spatial fluctuations are proportional to the averaged temperature gradient:

$$\widetilde{T_\alpha} = \overrightarrow{b} \cdot \overrightarrow{\text{grad}T}, \tag{5.19}$$

where $\overrightarrow{b}$ depends only on the porous geometry and the thermal conductivities. We can finally write:

$$(\rho c_v)^* \frac{\partial T}{\partial t} = \text{div}(\overline{\overline{\lambda}} \cdot \overrightarrow{\text{grad}T}), \tag{5.20}$$

with

$$\overline{\overline{\lambda}} = (\varepsilon \overline{\overline{\lambda_\alpha}} + (1-\varepsilon)\overline{\overline{\lambda_\sigma}}) + \frac{\overline{\overline{\lambda_\alpha}} - \overline{\overline{\lambda_\sigma}}}{V} \cdot \int_{S_{\alpha\sigma}} \overrightarrow{b} \cdot \overrightarrow{n}_{\alpha\sigma} dS. \tag{5.21}$$

The effective thermal conductivity depends on the porosity, the porous structure and the phase conductivities.

The order of magnitude of the effective thermal conductivity can spread from 10^{-5} W/m/K for multilayer insulators to 10^3 W/m/K for saturated a metallic matrix.

5.3 Estimation of effective conductivities

There exits several model to estimate the effective thermal conductivity of a porous media. They are included between two extreme configurations: parallel layers and series layers of fluid and solid.

A porous media composed of two phases and crossed by a thermal flux can be simplified in two ways. First we consider that it is a succession of solid and liquid layers in the heat flux direction. Then the layers are parallel to the heat flux. These two models are a large simplification of a porous media and correspond to bounds for effective thermal conductivity estimation. We denote as $\overrightarrow{\phi}$ the flux density vector crossing the porous media. The two layers are a fluid (conductivity λ_α) and a solid (conductivity λ_σ).

We first consider that the layer normal axis is parallel to the heat flux. It is the series arrangement. A way to estimate the effective conductivity consists in an electrical analogy. The effective thermal conductance is named G:

$$G = \lambda \frac{S}{L}, \tag{5.22}$$

where λ is the effective conductivity, S a cross-section of the sample (perpendicular to $\overrightarrow{\phi}$) and L the length of the sample in the $\overrightarrow{\phi}$ direction. Since we have a series arrangement, we can write:

$$\frac{1}{G} = \sum \frac{1}{G_\alpha} + \sum \frac{1}{G_\sigma}, \tag{5.23}$$

where G_α and G_σ are the conductance of one layer of the α-phase and σ-phase respectively, on a surface S. We denote as h_α and h_σ the thickness of each kind of layer. We have:

$$G_i = \lambda_i \frac{S}{h_i} \text{ with } i = \alpha, \sigma. \tag{5.24}$$

Consequently the total conductance can be expressed as:

$$\frac{1}{G} = \frac{1}{S\lambda_\alpha} \sum h_\alpha + \frac{1}{S\lambda_\sigma} \sum h_\sigma. \tag{5.25}$$

However, $\sum h_\alpha = L\varepsilon$ and $\sum h_\sigma = L(1-\varepsilon)$. Then we have:

$$G = \frac{S}{L}\frac{\lambda_\sigma\lambda_\alpha}{\varepsilon\lambda_\sigma + (1-\varepsilon)\lambda_\alpha} \tag{5.26}$$

Consequently we get :

$$\lambda = \frac{\lambda_\sigma\lambda_\alpha}{\varepsilon\lambda_\sigma + (1-\varepsilon)\lambda_\alpha} \Rightarrow \frac{\lambda}{\lambda_\alpha} = \frac{1}{\varepsilon + (1-\varepsilon)\dfrac{\lambda_\alpha}{\lambda_\sigma}}. \tag{5.27}$$

If $\lambda_\alpha \ll \lambda_\sigma$, we get a constant thermal conductivity ratio $\lambda/\lambda_\alpha \approx 1/\varepsilon$. If $\lambda_\alpha \gg \lambda_\sigma$, we get a linear thermal conductivity ratio $\lambda/\lambda_\alpha \approx \dfrac{\lambda_\sigma}{\lambda_\alpha}\dfrac{1}{1-\varepsilon}$.

We consider now a parallel arrangement where the layers are parallel to the heat flux imposed to the sample. In this case we can write:

$$G(W) = \frac{S}{L}\lambda = \sum G_\alpha + \sum G_\sigma = \lambda_\alpha \sum \frac{Wh_\alpha}{L} + \lambda_\sigma \sum \frac{Wh_\sigma}{L}, \tag{5.28}$$

with W an arbitrary length perpendicular to both heat flux and layers thickness. Furthermore we have $\sum Wh_\alpha = S\varepsilon$ and $\sum Wh_\sigma = S(1-\varepsilon)$. Consequently we have:

$$\lambda = \varepsilon\lambda_\alpha + (1-\varepsilon)\lambda_\sigma \Rightarrow \frac{\lambda}{\lambda_\alpha} = \varepsilon + (1-\varepsilon)\frac{\lambda_\sigma}{\lambda_\alpha}, \tag{5.29}$$

which gives an affine relation.

5.4 Convection in porous media

5.4.1 Homogeneization

As in a homogeneous media, porous media can be the place of convection phenomena, where heat is transported by fluid moves. There exist two kinds of convection: natural convection where the flow is induced only by temperature differences; and forced convection where flow is imposed from an external forcing.

We can demonstrate using volume averaging that the averaged fluid velocity and the average pressure are linked to the average temperature (under local equilibrium hypothesis $T = \langle T_\sigma\rangle^\sigma = \langle T_\alpha\rangle^\alpha$):

$$(\rho c_v)^* \frac{\partial T}{\partial t} + (\rho c_v)_\alpha \langle \overrightarrow{v}\rangle \cdot \overrightarrow{\text{grad}T} = \text{div}\left[(\overline{\overline{\lambda}} + \overline{\overline{\lambda_d}}) \cdot \overrightarrow{\text{grad}T}\right]; \tag{5.30}$$

$$\langle \overrightarrow{v}_\alpha\rangle = -\frac{\overline{\overline{k}}}{\eta}(\overrightarrow{\text{grad}}\langle P_\alpha\rangle^\alpha - \rho_\alpha \overrightarrow{g}); \tag{5.31}$$

$$\varepsilon\frac{\partial \rho_\alpha}{\partial t} + \text{div}(\rho_\alpha \langle \overrightarrow{v}_\alpha\rangle) = 0. \tag{5.32}$$

These equations are respectively heat equation, Darcy's law and mass conservation, both volume averaged.

$\overline{\overline{\lambda_d}}$ is the effective thermal conductivity tensor due to dispersion (induced by porous structure). The thermal diffusivity tensor can be defined as:

$$\overline{\overline{D}} = \frac{\overline{\overline{\lambda}} + \overline{\overline{\lambda_d}}}{(\rho c_v)_\alpha} = \frac{\overline{\overline{\lambda}}}{(\rho c_v)_\alpha} + \overline{\overline{D_d}}. \tag{5.33}$$

We can now define a thermal Péclet number:

$$Pe_{th} = \frac{\text{convection}}{\text{conduction}} = \frac{\langle \overrightarrow{v}_\alpha \rangle \ell_\alpha (\rho c_v)^*}{\varepsilon \lambda}, \tag{5.34}$$

where ℓ_α is the typical pore dimension. A large thermal Péclet number means that transport is mainly due to convection.

5.4.2 Dimensionless numbers for convection in porous media

To extract the two main control parameters of natural convection in porous media, we need to obtain the dimensionless equations of the system. Let us consider a saturated porous media included between two horizontal plates in $z = 0$ and $z = d$ at fixed temperatures T_1 and T_2 respectively, $T_1 > T_2$. The velocity field is $\overrightarrow{U} = \langle \overrightarrow{v} \rangle = (u, v, w)$, pressure is denoted as $P = \langle P_\alpha \rangle^\alpha$, temperature as $T = \langle T_\alpha \rangle^\alpha$. These quantities are linked via the model equations:

$$\begin{aligned}
\text{div}\overrightarrow{U} &= 0 && (5.35)\\
\rho &= \rho(T_0)[1 - \beta(T - T_0)] && (5.36)\\
\frac{d\overrightarrow{U}}{dt} &= -\frac{1}{\rho(T_0)}\overrightarrow{\text{grad}}P - \frac{\rho}{\rho(T_0)} g\overrightarrow{e_z} - \frac{\nu}{k}\overrightarrow{U} && (5.37)\\
\frac{dT}{dt} &= \kappa \Delta T. && (5.38)
\end{aligned}$$

ρ is the density of the fluid phase, β the thermal expansivity coefficient, T_0 a reference temperature, g the acceleration due to gravity, $\overrightarrow{e_z}$ the unit vertical vector, k the porous media permeability, ν the kinematic viscosity and $D = \dfrac{\lambda}{(\rho c_v)^*}$ the equivalent thermal diffusivity of the porous media. The boundary conditions are $T = T_1$ in $z = 0$, $T = T_2$ in $z = d$ and $w = 0$ in $z = 0, d$.

First, let us consider the conductive case, i.e. $\overrightarrow{U} = \overrightarrow{0}$ and stationarity. It leads to $\kappa \Delta T_c = 0$. Given the boundary conditions, by integrating twice we have:

$$T_c(z) = T_1 - \Gamma z. \tag{5.39}$$

The pressure profile can now be derived, using the boundary condition $P_c(0) = P_0$:

$$Pc(z) = P_0 - \rho(T_0) g (1 - \beta(T_0 - T_1) z - \frac{1}{2}\beta g \Gamma z^2. \tag{5.40}$$

We note $\theta = T - T_c$ and $P = P_c + \rho(T_0)\Pi$. All these quantities, except $\rho(T_0)$, depends on x, y, z, t. By replacing P and T from the initial system of equations, and having in mind the equations verified by T_c and P_c, we have:

$$\begin{aligned} \mathrm{div}\overrightarrow{U} &= 0 && (5.41)\\ \frac{d\overrightarrow{U}}{dt} &= -\overrightarrow{\mathrm{grad}}\Pi + \beta g\theta\overrightarrow{e_z} - \frac{\nu}{k}\overrightarrow{U} && (5.42)\\ \frac{d\theta}{dt} &= D\Delta\theta. && (5.43) \end{aligned}$$

We consider now small fluctuations around equilibrium state. By removing second-order terms, especially the convective part of the total derivatives $\frac{d}{dt}$, we get:

$$\begin{aligned} \mathrm{div}\overrightarrow{U} &= 0 && (5.44)\\ \frac{\partial\overrightarrow{U}}{\partial t} &= -\overrightarrow{\mathrm{grad}}\Pi + \beta g\theta\overrightarrow{e_z} - \frac{\nu}{k}\overrightarrow{U} && (5.45)\\ \frac{\partial\theta}{\partial t} &= \Gamma w + D\Delta\theta. && (5.46) \end{aligned}$$

The term Γw from the last equation comes from the z-component of the temperature gradient in the convective part of the total derivative of T.

To have dimensionless equations we fix the typical scales:

$$[L] = d,\ [\tau] = d^2/D,\ [\Theta] = T_1 - T_2,\ [U] = [L]/[\tau] \text{ and } [\Pi] = [U^2]. \quad (5.47)$$

Replacing $\overrightarrow{U}$ by $\overrightarrow{U}^*U$, Π by Π^*U^2, θ by $\theta^*\Theta$, and the time and lengths using their typical values L and τ, we get:

$$\begin{aligned} \mathrm{div}^*\overrightarrow{U}^* &= 0 && (5.48)\\ \frac{\partial\overrightarrow{U}^*}{\partial t^*} &= -\overrightarrow{\mathrm{grad}}^*\Pi^* + RaPr\theta^*\overrightarrow{e_z} - Pr\overrightarrow{U}^* && (5.49)\\ \frac{\partial\theta^*}{\partial t^*} &= w^* + \Delta^*\theta^*. && (5.50) \end{aligned}$$

The exponent * concerns dimensionless quantities. We have the dimensionless numbers:

$$Pr = \frac{\nu d^2}{kD} \qquad \text{and} \qquad Ra = \frac{\beta g dk(T_1 - T_2)}{D\nu}, \quad (5.51)$$

which are respectively the Rayleigh and Prandtl-like numbers.

We can also define the Nusselt number which compares the total heat flux to the hypothetical diffusive one. The Nusselt number follows power law when plotted as a function of the Rayleigh number.