

Introduction to Heat and Mass Transport in Porous Media

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ABSTRACT

Modeling transport in porous media requires to take into account multiple-scale aspects inherent to porous media structures. Several methodologies have been developed to upscale the equations at a lower-scale and to obtain upper-scale models. This question is reviewed based on a simple heat conduction problem. This is used to present briefly: volume averaging, homogenization, stochastic approaches, and various variants. Following the guidelines provided by volume averaging, the problem of the emergence of macro-scale equations for momentum and energy balance is discussed, with the emphasis on the existence of different models depending on pore-scale physical properties (dimensionless parameters, various time and length-scale ratios). Finally, extensions to more complicated problems of heat transfer in porous media, characterized by various couplings between transport problems, are briefly discussed: coupling with mass diffusion, effect of heat sources, boiling, etc.

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1.0 INTRODUCTION

Heat and mass transfer in porous media is central to many applications involving industrial devices (chemical engineering, heat exchangers, nuclear reactor, etc.) as well as complex geological formations (CO₂ storage, in situ combustion and pyrolysis, geothermal applications, etc.). Most of the time, such transport problems are characterized by highly non-linear couplings and many different scales involved. A typical multi-scale feature is illustrated in Fig. 1, which represents a typical porous medium two-scale description. The lower-scale is the pore-scale where phases may be treated as separated continua, here a β -phase flowing in a solid structure made of a σ -phase, with pore-scale characteristic lengths l_β and l_σ . The upper-scale or macro-scale calls for an effective representation characterized by variations of the variables at a scale L . To be applicable, such a macro-scale representation requires the validity of a separation of scale assumption implying $l_\beta, l_\sigma \ll r_0 \ll L$ where r_0 is some intermediated scale at which macro-scale variables are defined. This latter scale is related to the existence of a Representative Elementary Volume which has been discussed at length in the literature ([1, 2]). In the sequel of this presentation, it will be assumed that all scales involved are nicely separated, as it is illustrated Figure 2 but the reader must not forget that this does not happen all the time. If L is too close to l , direct numerical simulation or meso-scale approaches must be used, such as network modeling ([3]). Another class of porous media which will not be considered in this lecture calls also for specific approaches: those with a fractal structure over a large range of scales ([4]).

The introduction of relevant macro-scale models is one of the major problem of porous media physics. Of course, one may introduce ad hoc or heuristic models, and, indeed, this is the case for many of the classical macro-scale models used in the engineering practice, starting with the classical Darcy’s law [5]. However, it is often more reliable to have at its disposal a comprehensive framework that links explicitly the pore-scale physics to a macro-scale theory. This provides a strong basis for developing correct physical models, but it also offers a guidance for developing new, original models for surging problems. Because of the problem complexity due to the multi-scale aspects, there is not a single route from one pore-scale problem to a macro-scale model. Two major issues are encountered:

- the interplay between different transport mechanisms and the potential high contrast of transport properties (such as diffusivities for instance) lead to several macro-scale behaviors requiring specific macro-scale models. This is illustrated in Sec. 4.0 with the discussion about non-equilibrium and equilibrium models,
- Similarly, it is not surprising to find that many different methods have been developed to deal with the upscaling aspects.

This lecture offers a brief *overview* of these two problems and provides a short *introduction* to some of the classical transport models available with a discussion on their physical meaning from a multiple-scale perspective. The first section introduces briefly some available upscaling techniques. Next, the potential for different

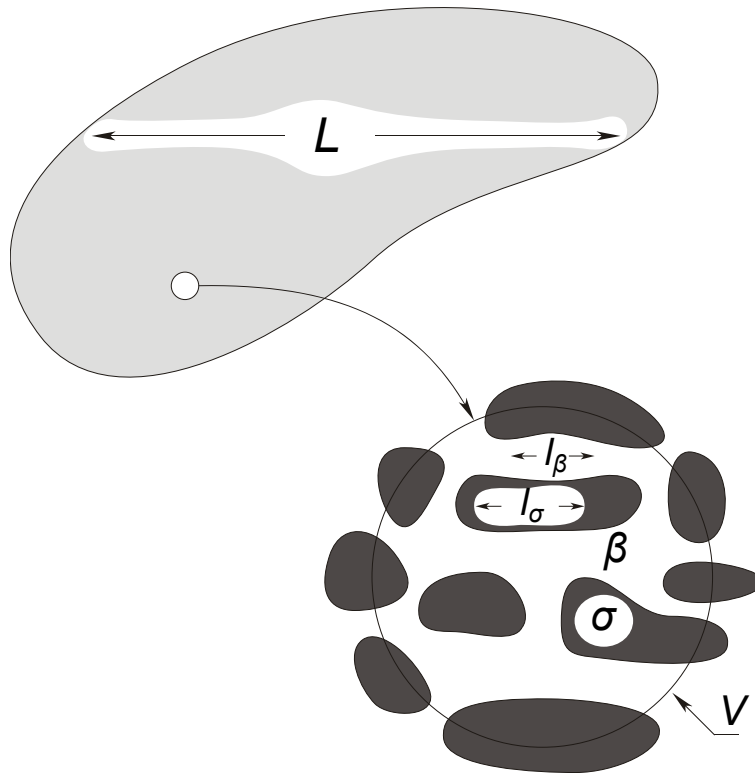


Figure 1: Multiple-scale description of a porous medium.

macro-scale models will be illustrated for a classical porous medium heat and mass transfer problem. Finally, indications will be given on open or modern problems which are the subject of current research, especially in the area of heat transfer in porous media.

2.0 UPSCALING METHODOLOGIES: A BRIEF OVERVIEW

To illustrate the various methodologies, let us start with a simple, steady-state heat transfer problem over a medium with a l -scale heterogeneous but continuous thermal conductivity, $\mathbf{k}(\mathbf{x})$. The pore-scale equation is written as

$$\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla T) = 0 \quad (1)$$

where T is the temperature. This equation is mathematically equivalent to the problem of a Darcy flow in a heterogeneous porous medium or to a classical mass diffusion problem. Therefore, some of the cited papers in the following developments are in fact connected to these latter problems and not heat transfer. This meaningless difference is not stressed in the following discussion. Most of the material used in this introduction is taken from [6–8].

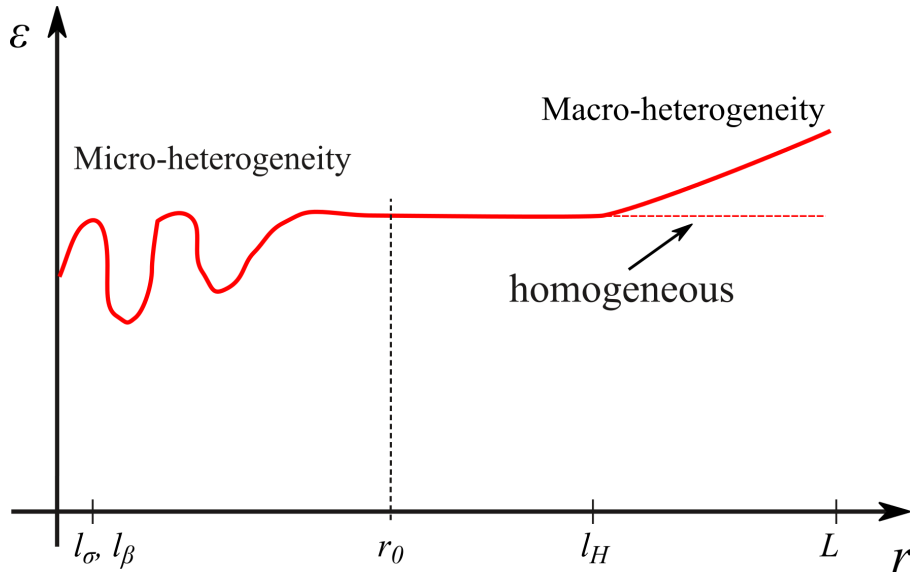


Figure 2: Schematic representation of the separation of scales

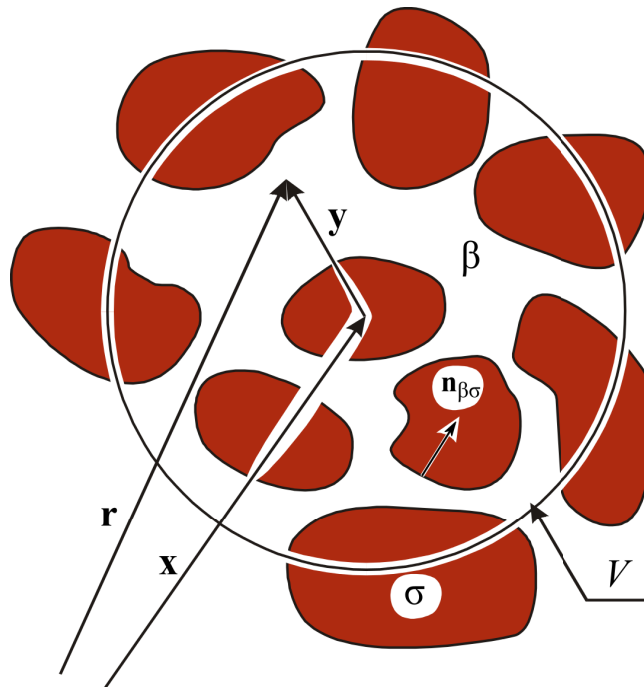


Figure 3: Averaging Volume

2.1 A physicist view through volume averaging

How to define macro-scale variables and how to obtain macro-scale equations? Macro-scale variables can be thought of as regularized fields of the micro-scale fields. This is not surprising that the idea of regularization through some spatial convolution was originally proposed as a designated tool to achieve this task ([9–12] and many others). In this framework, the macro-scale temperature field is defined by

$$\langle T \rangle (\mathbf{x}, t) = \frac{1}{V} \int_{\mathbf{r} \in V(\mathbf{x})} T(\mathbf{r}) dV_{\mathbf{r}} \quad (2)$$

where $V(\mathbf{x})$ is a volume centered at \mathbf{x} and of volume V , as it is illustrated Fig. 3. The regularization process through spatial averaging may require special attention if used with simple kernel functions such as the one involved in Eq. (2). This point is not discussed in this paper and the reader is referred to [9, 12, 13] and the series of paper [14–18] for a better understanding of the problem. The macro-scale equation can be obtained from averaging of the pore-scale equation and this leads to

$$\nabla \cdot \langle \mathbf{k}(\mathbf{x}) \cdot \nabla T \rangle = 0 \quad (3)$$

which cannot be readily put under a closed form, i.e., an equation involving only $\langle T \rangle$ as the independent variable with some *effective* property describing the macro-scale behavior. A work-flow to achieve this goal makes use of the following steps [19]:

Step 1: define temperature deviation

$$T = \langle T \rangle + \tilde{T} \quad (4)$$

Step 2: develop averaged equation

$$\nabla \cdot \langle \mathbf{k}(\mathbf{x}) \cdot (\nabla \langle T \rangle + \nabla \tilde{T}) \rangle = 0 \quad (5)$$

Step 3: obtain micro-scale governing equation for the deviation

$$\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla \tilde{T}) = -\nabla \cdot (\mathbf{k}(\mathbf{x}) \cdot \nabla \langle T \rangle) \quad (6)$$

Step 4: develop a *closure*, i.e., solve in an approximate manner (using approximations based on the separation of scales) the coupled micro and macro-scale problem. From the mathematical structure of Eqs. 5 and 6, one may propose the following mapping of the gradient of the macro-scale temperature onto the temperature deviation

$$\tilde{T} = \mathbf{b} \cdot \nabla \langle T \rangle + \dots \quad (7)$$

where the mapping vector \mathbf{b} is determined by

$$\nabla \cdot (\mathbf{k} \cdot \nabla \mathbf{b}) = -\nabla \cdot \tilde{\mathbf{k}} \quad (8)$$

completed by

$$\langle \mathbf{b} \rangle = 0 \quad ; \quad \mathbf{b}(\mathbf{x} + \mathbf{l}) = \mathbf{b}(\mathbf{x}) \quad i = 1, 2, 3 \quad (9)$$

where the first equation ensures that the average of the deviation is zero and the last equation corresponds to periodicity conditions. Periodicity conditions work well for true periodic porous media. Most media are not periodic (randomly generated media, tomographic images, ...) and the boundary conditions must be adapted (see discussion of this problem in [20]).

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Step 5: Obtain a closed form of the macro-scale equation by replacing the deviations in the averaged equation (Eq. 5) by its mapping (Eq. 7), i.e., one obtains

$$\nabla \cdot (\mathbf{K}_{eff} \cdot \nabla \langle T \rangle) = 0 \quad (10)$$

in which the *effective property*, here a thermal conductivity tensor, is given by

$$\mathbf{K}_{eff} = \langle \mathbf{k} \cdot (\mathbf{I} + \nabla \mathbf{b}) \rangle \quad (11)$$

The upscaling method provides not only the form of the equation compatible with the assumptions made, but also local problems (often named as *closure problems*) for calculating the effective property through the knowledge of pore-scale characteristics. While such calculations were considered in the past as too heavy and impractical, given the poor access to pore-scale characteristic and the computational requirements, this is now becoming more of a routine thanks to bigger computers and tools like CT-scanners ([21]). Indeed, several commercial softwares for CT-scan treatment propose toolboxes to compute the most simple effective properties (diffusivity, permeability, ...).

The above work-flow is a schematic presentation in the case of a simple problem. A more comprehensive presentation can be found in [19]. Other techniques were devised to interpret the additional terms that appear when balance equations are averaged. For instance, this can be achieved heuristically ([11, 22]) or in recognition of the physical notions of tortuosity, dispersion terms, etc... Intermediate approaches have been used to interpret micro-scale numerical simulations and to propose new forms of macro-scale equations (e.g. in [23, 24]), which offers, through a less complex closure, a possible way of dealing with complicated coupled problems.

2.2 Other methodologies

Different methodologies have been proposed to achieve the same goal, which differ by many different aspects. In particular, one should look at the operator defining the macro-scale variable. A brief overview of the major branches is presented below.

Homogenization theory

Asymptotic methods have been used in mathematics to study differential operators involving rapidly oscillating coefficients. The development of the homogenization theory for porous media problems follows this idea. The macro-scale fields are defined in the sense of some limit with respect to a small number, ϵ , characteristic of the separation of scale, i.e., $\frac{l}{L}$. This idea can be developed mathematically speaking following different routes. This is not the objective of this lecture to provide a complete picture, and, for simplicity, the development will be outlined using asymptotic expansions for periodic domains, as in [25–31, 31, 32] and many other contributions. One may refer to [33–35] for the presentation of different, less restrictive views. Basically, the temperature field will be looked at in terms of a multi-scale expansion involving \mathbf{x} and \mathbf{y} treated as independent variables in the limit $\epsilon \rightarrow 0$ such as

$$T(\mathbf{x}) = \sum_i T_i \left(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon} \right) \epsilon^i \quad (12)$$

where the first term will play the role of the macro-scale variable and the subsequent terms the role of the deviation, like in Eq. (4). The perturbation analysis gives the following results (here one assumes that $\mathbf{k}(\mathbf{x}, \mathbf{y}) = \mathbf{k}(\mathbf{y})$).

The ϵ^{-2} term gives $T_0(\mathbf{x}, \mathbf{y}) = T_0(\mathbf{x})$, while the term ϵ^{-1} gives a local (closure) problem such as

$$\nabla_{\mathbf{y}} \cdot (\mathbf{k} \cdot \nabla_{\mathbf{y}} T_1) + \nabla_{\mathbf{y}} \cdot (\mathbf{k} \cdot \nabla_{\mathbf{x}} T_0) = 0 \quad (13)$$

which suggests a solution of the form

$$T_1(\mathbf{x}, \mathbf{y}) = \mathbf{b}(\mathbf{y}) \cdot \nabla_{\mathbf{x}} T_0(\mathbf{x}) \quad (14)$$

with the periodic mapping vector $\mathbf{b}(\mathbf{y})$ obeying

$$\nabla_{\mathbf{y}} \cdot (\mathbf{k} \cdot \nabla_{\mathbf{y}} \mathbf{b}) = -\nabla_{\mathbf{y}} \cdot \mathbf{k} \quad ; \quad \langle \mathbf{b} \rangle = 0 \quad ; \quad \mathbf{b}(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}(\mathbf{x}) \quad i = 1, 2, 3 \quad (15)$$

The ϵ^0 term, after integration over a unit cell, gives the macro-scale equation

$$\nabla_{\mathbf{x}} \cdot (\mathbf{K}_{eff} \cdot \nabla_{\mathbf{x}} T_0) = 0 \quad (16)$$

where the effective thermal conductivity is given by

$$\mathbf{K}_{eff} = \langle \mathbf{k} \cdot (\mathbf{I} + \nabla_{\mathbf{y}} \mathbf{b}) \rangle \quad (17)$$

This is beyond the scope of this paper to give a complete comparison between the two methods. The reader may refer to a preliminary work by [36] and a more thorough analysis by [6, 7]. One sees from the two developments that:

- the operational definition of the macro-scale variables is different, while one may recognize that $\langle T \rangle = \langle \sum_i T_i(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon}) \epsilon^i \rangle = T_0$,
- closure is based on a perturbation analysis making use of the separation of scales, through order of estimates analysis or through the manipulation of the "independent" variables (in a limit sense) \mathbf{x} and \mathbf{y} ,
- in both approaches, the macro-scale equation is obtained after averaging the micro-scale equation, taking into account the separation of scales.

Given the fact that both methods solve the same deterministic problem, it is not surprising that the perturbation analysis gives the same "closure" and the same macro-scale equation.

Stochastic method

A non deterministic point of view has been adopted by many scientists, especially in the field of hydrogeology ([37–40]). Because of the complex and more or less disordered heterogeneities found in natural media, the actual porous medium is seen as a particular realization of a stochastic ensemble and, therefore, the macro-scale variable is defined as an expectation, i.e.

$$T^e = E(T) \quad (18)$$

There is not a straightforward connection between $T^e = E(T)$ and $\langle T \rangle$. However, the link between the stochastic point of view and spatial averaging comes from an ergodicity assumption which is most often considered when building the ensemble statistical properties (see a discussion in [41]). In this framework, the thermal conductivity in the heat equation becomes a random space function and the heat equation itself is a stochastic PDE. Many different techniques are available to get solutions of the corresponding stochastic problem, and they do not compare necessarily with the methods described above for volume averaging with closure or for the homogenization theory. However, some methods make use of a perturbation analysis in terms of the covariance of k (see [39, 42]), which is reminiscent of the way a "closure" is obtained with the previously introduced

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upscaling methods. One may refer to [43] for a comparison between the stochastic analysis of the problem of dispersion in [44] and results obtained with the use of a volume averaging theory from [45].

A less limited approach in terms of the thermal conductivity variance corresponds to the self-consistent method and the many variants also called effective-medium theories in which the effective conductivity is built from the calculation of the interaction between an inclusion embedded into a homogeneous medium having the effective transport property ([39]).

While this also can be obtained from the closure problems for the method of volume averaging or the homogenization theory, stochastic analysis allows to develop in a quite straightforward manner bounds for the effective thermal conductivity. One easily obtain (see [39], chap. 2) by looking at the expectation for the flow energy that

$$K_H \leq K_{eff} \leq K_A \quad (19)$$

where K_H and K_A are the harmonic mean and arithmetic mean respectively of the pore-scale thermal conductivity. This question of bounds for the effective properties is of a great practical importance and is discussed a little bit further in Sec. 4.2.1.

Variants

Each method has several variants, as indicated before in the case of the homogenization theory. The method of volume averaging has also many variants. For example, [9, 46] justify Darcy's law using the theoretical framework of irreversible thermodynamics. The idea that macroscale models should be compatible with the principles of thermodynamics was not new ([47–49]), but the coupling with volume averaging produced a specific methodology used by several authors (for instance [50], [51], ...). Such a methodology is also reminiscent of the theory of mixtures (see [52]). While there is not a specific closure, i.e., a deterministic mapping between macro-scale variables and deviations, the structure of the macro-scale models for complex, non-linear coupled systems may be constrained by the method, which in turn provides interesting guidelines for the interpretation of experiments or numerical simulations. The method of moments for spatially periodic media, as developed in [53, 54], bears also some resemblance with the two-scale methods discussed in Sec. 2.1 and 2.2.

Many other ideas have been tested and this is beyond the scope of this lecture to provide a comprehensive analysis. This short comparison of several methods put the emphasis on:

- the definition of macro-scales variables,
- the way the coupled micro- and macro-scale problems are approximated,
- the existence of an explicit closure, which provides a straightforward way of calculating effective properties from the micro-scale characteristics.

In the next sections, results are provided for a classical heat and mass transfer in porous media problem. The steps for the upscaling developments will not be detailed heavily but rather the emphasis will be put on several fundamental questions, in particular the question of the *existence of various models* for the same mathematical problem, depending on the flow properties and pore-scale characteristics. This is an intricate question which is often overlooked and may result in misleading recommendations.

3.0 REVIEW OF MACRO-SCALE MOMENTUM BALANCE EQUATIONS

The pore-scale problem under consideration may be written for a Newtonian fluid with constant density and viscosity as

$$\nabla \cdot \mathbf{v}_\beta = 0 \text{ in } V_\beta \quad (20)$$

$$\rho_\beta \frac{\partial \mathbf{v}_\beta}{\partial t} + \rho_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{v}_\beta = -\nabla p_\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \mathbf{v}_\beta \text{ in } V_\beta \quad (21)$$

$$\text{B.C.1} \quad \mathbf{v}_\beta = 0 \quad \text{at } A_{\beta\sigma} \quad (22)$$

The upscaling problem has received a lot of attention in the literature. One may distinguish various types of flow patterns, depending on the pore-scale Reynolds number that may be defined as

$$\text{Re} = \frac{\rho_\beta U_r l_\beta}{\mu_\beta} \quad (23)$$

where U_r is a reference velocity taken usually as the intrinsic average velocity which will be defined later. The sequence of pore-scale behavior depends on the Reynolds number as will be discussed below. For now on, let us look at some details of the problem using the method of volume averaging as a guideline.

3.1 Miscellaneous definitions and theorems

First, the definition of averages presented in Eq. 2 must be adapted to fields which are only defined in the β -phase. The average of a given field ψ_β is

$$\langle \psi_\beta \rangle = \frac{1}{V} \int_{V_\beta} \psi_\beta dV \quad (24)$$

which, when applied to the phase indicator γ_β

$$\gamma_\beta = \begin{cases} 1 & M \in V_\beta \\ 0 & M \notin V_\beta \end{cases} \quad (25)$$

gives

$$\varepsilon_\beta = \langle \gamma_\beta \rangle = \frac{1}{V} \int_{V_\beta} dV = \frac{V_\beta}{V} \quad (26)$$

which is called the β -phase volume fraction, equal to the medium porosity, ε , in the case of a single phase flow. One has the obvious relation

$$\varepsilon_\beta + \varepsilon_\sigma = 1 \quad (27)$$

From that the porosity is also given by

$$\varepsilon = 1 - \varepsilon_\sigma \quad (28)$$

and the β -phase saturation is defined as

$$\varepsilon_\beta = \varepsilon S_\beta \quad (29)$$

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with $S_\beta \in [0, 1]$. It is also interesting to introduce an intrinsic phase average, $\langle \psi_\beta \rangle^\beta$, as

$$\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta \quad (30)$$

Applying these definitions to the velocity and pressure fields one may introduce the following notations

$$\mathbf{V}_\beta = \langle \mathbf{v}_\beta \rangle = \varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta = \varepsilon_\beta \mathbf{U}_\beta \quad (31)$$

where \mathbf{V}_β is called the superficial or filtration velocity and \mathbf{U}_β is the intrinsic average velocity for the β -phase. The developments make use of the intrinsic average pressure which will be denoted as

$$P_\beta = \langle p_\beta \rangle^\beta \quad (32)$$

The mathematical development makes extensive use of the classical averaging theorems (see [12] for a proof using the theory of distribution) given by

$$\langle \nabla \psi_\beta \rangle = \nabla \langle \psi_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_\beta dA \quad (33a)$$

$$\langle \nabla \cdot \mathbf{A}_\beta \rangle = \nabla \cdot \langle \mathbf{A}_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_\beta dA \quad (33b)$$

$$\left\langle \frac{\partial \psi_\beta}{\partial t} \right\rangle = \frac{\partial \langle \psi_\beta \rangle}{\partial t} - \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} \psi_\beta dA \quad (33c)$$

where $\mathbf{n}_{\beta\sigma}$ is the normal to the interface $A_{\beta\sigma}$, $\mathbf{w}_{\beta\sigma}$ the interface velocity.

3.2 Macro-scale momentum equations for one-phase flow

Using the upscaling "algorithm" outlined in Sec. 2.1, one obtains the following unclosed averaged equations

$$\nabla \cdot \langle \mathbf{v}_\beta \rangle = 0 \quad (34)$$

$$\begin{aligned} & \frac{\partial \rho_\beta \langle \mathbf{v}_\beta \rangle}{\partial t} + \rho_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta + \nabla \cdot (\rho_\beta \langle \tilde{\mathbf{v}}_\beta \tilde{\mathbf{v}}_\beta \rangle) = \\ & -\varepsilon_\beta \nabla \langle p_\beta \rangle^\beta + \varepsilon_\beta \rho_\beta \mathbf{g} + \underbrace{\mu_\beta \nabla^2 \langle \mathbf{v}_\beta \rangle - \mu_\beta \nabla \varepsilon_\beta \cdot \nabla \langle \mathbf{v}_\beta \rangle^\beta}_{\text{Brinkman terms}} + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA \end{aligned} \quad (35)$$

which must be solved with the pore-scale equations.

Many practical applications are characterized by creeping flows observed when inertia terms may be neglected at low Reynolds number. In this case the momentum equation degenerates into Stokes equation and the inertia terms are put to zero in Eq. 35. In addition, the Brinkman terms are often neglected in this equation on the basis that they correspond to variations at the Darcy-scale and hence they are small compared to the drag term due to the solid phase [55]. The pore-scale equations written in terms of averaged values and deviations lead to the following equations

$$\nabla \cdot (\tilde{\mathbf{v}}_\beta) = -\nabla \cdot \langle \mathbf{v}_\beta \rangle^\beta \approx 0 \quad (36)$$

$$0 = -\nabla \tilde{p}_\beta + \mu_\beta \nabla^2 \tilde{\mathbf{v}} - \varepsilon_\beta^{-1} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\tilde{p}_\beta \mathbf{I} + \mu_\beta \nabla \tilde{\mathbf{v}}_\beta) dA \quad (37)$$

$$\text{B.C. 1 } \tilde{\mathbf{v}} = -\langle \mathbf{v}_\beta \rangle^\beta \text{ sur } A_{\beta\sigma} \quad (38)$$

The final coupled system of linear equations may be solved approximatively by introducing the following mapping between the deviations and averaged values [55]

$$\tilde{p}_\beta = \mu_\beta \mathbf{b} \cdot \langle \mathbf{v}_\beta \rangle^\beta + .. ; \tilde{\mathbf{v}} = \mathbf{B} \cdot \langle \mathbf{v}_\beta \rangle^\beta + .. \quad (39)$$

Introducing this mapping into the pore-scale equations gives the following *closure problem*

$$\nabla \cdot \mathbf{B} = 0 \quad (40)$$

$$-\nabla \mathbf{b} + \nabla^2 \mathbf{B} = \varepsilon_\beta^{-1} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I} \mathbf{b} + \nabla \mathbf{B}) dA \quad (41)$$

$$\mathbf{B} = -\mathbf{I} \text{ sur } A_{\beta\sigma}, \langle \mathbf{b} \rangle^\beta = 0 \quad (42)$$

$$\mathbf{b}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}(\mathbf{r}) \quad \mathbf{B}(\mathbf{r} + \mathbf{l}_i) = \mathbf{B}(\mathbf{r}) \quad (43)$$

The above problem leads also to the property

$$\langle \mathbf{B} \rangle^\beta = 0 \quad (44)$$

As a consequence, the averaged equation may be written

$$\langle \mathbf{v}_\beta \rangle = -\frac{1}{\mu_\beta} \mathbf{K} \cdot (\nabla \langle p_\beta \rangle^\beta - \rho_\beta \mathbf{g}) \quad (45)$$

or, with the proposed notations,

$$\mathbf{V}_\beta = -\frac{1}{\mu_\beta} \mathbf{K} \cdot (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (46)$$

where the permeability tensor, \mathbf{K} , is given by

$$\mathbf{K}^{-1} = -\varepsilon_\beta^{-2} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot (-\mathbf{I} \mathbf{b} + \nabla \mathbf{B}) dA \quad (47)$$

One recognizes in Eq. 46 the well known Darcy equation which was originally introduced heuristically by Darcy in 1856 [5]. Increasing the Reynolds number, inertia terms start to play a dominant role. The way the relation pressure drop/velocity departs from the linear Darcian regime has been the object of many discussions and controversies. Staying in a laminar regime, one needs to add an extra, inertia term, in the macro-scale equation. Generally, it can be written as

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \mathbf{K}^{-1} \cdot \mathbf{V}_\beta - \mathbf{F}(\mathbf{V}_\beta) \cdot \mathbf{V}_\beta \quad (48)$$

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where the term $\mathbf{F}(\mathbf{V}_\beta) \cdot \mathbf{V}_\beta$ is called a generalized Forchheimer term in reference to the work of [56]. If one looks at the upscaling problem in terms of an asymptotic expansion with the Reynolds number, the first correction to Darcy's law, i.e., at sufficiently low Reynolds number in a regime called weak inertia regime, is cubic in terms of the velocity, i.e., $\mathbf{F}(\mathbf{V}_\beta) \sim \|\langle \mathbf{v}_\beta \rangle\|^2$ [57–61]. If one increases the Reynolds number but still keeping a laminar flow, inertia effects may be *approximated* macroscopically by a quadratic term, i.e., $\mathbf{F}(\mathbf{V}_\beta) \sim \|\langle \mathbf{v}_\beta \rangle\|$. This is supported by experimental data [56, 62–66] as well as numerical predictions [60, 67].

While the above theoretical discussions suggest the potential existence of anisotropy effects for the Forchheimer terms, the engineering practice relies on simpler expressions, in particular the use of Ergun's equation [62] which reads

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta K^{-1} \mathbf{V}_\beta - \rho_\beta \eta^{-1} \|\mathbf{V}_\beta\| \mathbf{V}_\beta \quad (49)$$

where η is called the *passability*. Based on collected experimental data, Ergun proposed correlations for K and η in the case of packed beds which are still very popular in the engineering practice:

$$K = \frac{\varepsilon^3 d^2}{h_K (1 - \varepsilon)^2} \quad ; \quad \eta = \frac{\varepsilon^3 d}{h_\eta (1 - \varepsilon)} \quad (50)$$

where d is the equivalent particle diameter and $h_K = 150$ and $h_\eta = 1.75$.

If a generalized Forchheimer equation can be reasonably used to describe strong inertia effects in laminar regimes, this model is also used in the case of unit-cell localized or periodic turbulence, has shown theoretically in [68, 69]. Turbulence is not always of periodic type [70] and several attempts have been made to develop *macro-scale* turbulence models. Two sequential schemes have been discussed in the literature, as illustrated below

$$\text{I. } \mathbf{v}_\beta \rightarrow \langle \mathbf{v}_\beta \rangle \rightarrow \overline{\langle \mathbf{v}_\beta \rangle} \quad (51)$$

$$\text{II. } \mathbf{v}_\beta \rightarrow \overline{\mathbf{v}_\beta} (\text{RANS}, \dots) \rightarrow \langle \overline{\mathbf{v}_\beta} \rangle \quad (52)$$

Scheme I, favored by [71, 72] among others, involves a first spatial averaging. It is assumed that the closed macro-scale equations are of a generalized Forchheimer type, an assumption which is difficult to assess. This is followed by a time averaging procedure. Most researchers follow scheme II. In this case, it is assumed that the Navier-Stokes equations may be time averaged and the resulting equations are subsequently spatially averaged ([73, 74]). In both cases, the possibility of a decoupled closure for both types of averages is difficult to justify. The result is some sort of effective RANS macro-scale model. A complete validation either through experiments or through numerical modeling is still an open problem. The need for such model is also a matter of evaluation. It is interesting to notice that it has been observed, based on direct numerical simulations, that turbulence generated in a fluid layer or at the interface between fluid and porous layers, may indeed penetrate several unit cells into the porous domain and that in this area a porous medium turbulence model is needed ([75]).

3.3 Macro-scale momentum equations for two-phase flow

The case of two-phase flows is very important in many applications (petroleum and chemical engineering, nuclear safety, ...). A full development of this problem will not be proposed here. However, this is necessary to understand the major aspects which are summarized below, in order to make proper use of the various models

available. The pore-scale problems involves mass and momentum balance equations for both phases denoted β and γ . They are coupled through the boundary condition at the fluid-fluid interface, namely

$$\begin{aligned} & -\mathbf{n}_{\beta\gamma} p_\beta + \mu_\beta \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T \right) = \\ & -\mathbf{n}_{\beta\gamma} p_\gamma + \mu_\gamma \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\gamma + (\nabla \mathbf{v}_\gamma)^T \right) + 2\sigma H_{\beta\gamma} \mathbf{n}_{\beta\gamma} \text{ at } A_{\beta\gamma} \end{aligned} \quad (53)$$

where σ is the interfacial tension and $H_{\beta\gamma}$ the interface curvature. In the framework of the upscaling theory, it can be transformed into

$$\begin{aligned} & -\mathbf{n}_{\beta\gamma} P_\beta|_{\mathbf{x}} - \mathbf{n}_{\beta\gamma} \mathbf{y}_\beta \cdot \nabla P_\beta|_{\mathbf{x}} - \dots - \mathbf{n}_{\beta\gamma} \tilde{p}_\beta + \mu_\beta \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\beta + (\nabla \mathbf{v}_\beta)^T \right) = \\ & -\mathbf{n}_{\beta\gamma} P_\gamma|_{\mathbf{x}} - \mathbf{n}_{\beta\gamma} \mathbf{y}_\gamma \cdot \nabla P_\gamma|_{\mathbf{x}} - \dots - \mathbf{n}_{\beta\gamma} \tilde{p}_\gamma + \mu_\gamma \mathbf{n}_{\beta\gamma} \cdot \left(\nabla \mathbf{v}_\gamma + (\nabla \mathbf{v}_\gamma)^T \right) + 2\sigma H_{\beta\gamma} \mathbf{n}_{\beta\gamma} \text{ at } A_{\beta\gamma} \end{aligned} \quad (54)$$

This condition can be replaced, for small capillary and Bond numbers defined as

$$\text{Ca} = \frac{\mu_r U_r}{\sigma} \quad ; \quad \text{Bo} = \frac{|(\rho_\beta - \rho_\gamma) g| r_0^2}{\sigma} \quad (55)$$

by

$$P_\gamma|_{\mathbf{x}} - P_\beta|_{\mathbf{x}} = 2\sigma H_{\beta\gamma} \quad (56)$$

Under these conditions, the interface curvature is locally constant and quasi-static and this leads to the introduction of a macro-scale *capillary pressure* condition expressed as

$$P_\gamma - P_\beta = p_c(S_\beta, \dots) \quad (57)$$

This line of reasoning together with the assumption of creeping flows (i.e., very low Reynolds number) is at the base of the heuristic generalized Darcy's law model classically used in engineering practice, often attributed to [76]. Besides the capillary pressure relationship one has

$$\frac{\partial \varepsilon S_\beta}{\partial t} + \nabla \cdot \mathbf{V}_\beta = 0 \quad (58)$$

$$\mathbf{V}_\beta = -\frac{1}{\mu_\beta} \mathbf{K}_\beta \cdot (\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (59)$$

$$\frac{\partial \varepsilon S_\gamma}{\partial t} + \nabla \cdot \mathbf{V}_\gamma = 0 \quad (60)$$

$$\mathbf{V}_\gamma = -\frac{1}{\mu_\gamma} \mathbf{K}_\gamma \cdot (\nabla P_\gamma - \rho_\gamma \mathbf{g}) \quad (61)$$

with the phase permeabilities generally written in terms of relative permeabilities in the following manner

$$\mathbf{K}_\beta = \mathbf{K} k_{r\beta}(S_\beta) \quad ; \quad \mathbf{K}_\gamma = \mathbf{K} k_{r\gamma}(S_\gamma) \quad (62)$$

The reader must be warned that the introduction of scalar relative permeabilities is not justified in all cases as illustrated in [77, 78]. Finally, one must not forget the obvious condition

$$S_\beta + S_\gamma = 1 \quad (63)$$

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The triple line or wettability effects must be taken into account in the analysis. In the classical model, it essentially plays a role in the non-linear capillary and relative permeability relationships.

If one keeps the viscosity terms in the boundary condition Eq. 54 while making the assumption of quasi-staticity, small Bond and Reynolds numbers, one finds [79–83, ...] slightly different macro-scale momentum balance equations with cross terms which may be written in the following way

$$\mathbf{V}_\alpha = -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha \cdot (\nabla P_\alpha - \rho_\alpha \mathbf{g}) + \mathbf{K}_{\alpha\kappa} \cdot \mathbf{V}_\kappa \quad \alpha, \kappa = \beta, \gamma \quad \alpha \neq \kappa \quad (64)$$

These terms have been the subject of long controversies about their relative importance [84, 85, ...] and they are so far discarded in most applications, in particular petroleum engineering. They account however for some drag force that is required to explain the retention of water observed in a vertical column subject to an upward gas flow in the case of a high permeability medium [61, 86–89]. In particular, this effect is important in chemical engineering or in nuclear safety (debris bed reflooding) applications. One may want to remove the drastic assumptions made previously, in particular quasi-staticity, and this has led to various proposals which are not discussed in detail here [90–93, ...]. It must be emphasized, however, that they have the potential to explain more dynamic behavior of multiphase flow in porous media such as dependence of effective properties with velocity, saturation evolution, etc...

When the Reynolds number becomes large, inertia effects start to play a significant role. This has also received a lot of attention in the literature. The simplest proposal to take these effects into account is based on a generalized Ergun's law such as [94]

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K} \frac{1}{k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta \quad (65)$$

where $k_{r\beta}$ is the relative permeability of the β -phase and η_β its relative passability. These parameters are often assigned the following forms

$$k_{r\beta} = (1 - S_\gamma)^n \quad ; \quad \eta_\beta = (1 - S_\gamma)^m \quad (66)$$

$$k_{r\gamma} = S_\gamma^p \quad ; \quad \eta_\gamma = S_\gamma^q \quad (67)$$

with the exponents taking different values [95–97, ...]. While this form may account for the pressure drop increase due to inertia effects, it does not fully take into account the drag between both phases which leads to a retention of water due to counter-current flow higher than the one associated to capillary pressure trapping at irreducible saturation. Several proposals have been introduced to take this effect into account, like for instance the model proposed by [88]

$$0 = -\nabla P_\beta + \rho_\beta \mathbf{g} - \mu_\beta \frac{1}{K} \frac{1}{k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta + \frac{\mathbf{F}_{\beta\gamma}^S}{S_\beta} \quad (68)$$

$$0 = -\nabla P_\gamma + \rho_\gamma \mathbf{g} - \mu_\beta \frac{1}{K} \frac{1}{k_{r\beta}} \mathbf{V}_\beta - \frac{\rho_\beta}{\eta \eta_\beta} \|\mathbf{V}_\beta\| \mathbf{V}_\beta - \frac{\mathbf{F}_{\beta\gamma}^S}{1 - S_\beta} \quad (69)$$

A generalized form of two-phase flow equations accounting for cross terms and inertia effects can be obtained theoretically through upscaling [98], it reads

$$\begin{aligned} \mathbf{V}_\alpha = & -\frac{1}{\mu_\alpha} \mathbf{K}_\alpha \cdot (\nabla P_\alpha - \rho_\alpha \mathbf{g}) - \mathbf{F}_{\alpha\alpha} \cdot \mathbf{V}_\alpha \\ & + \mathbf{K}_{\alpha\kappa} \cdot \mathbf{V}_\kappa - \mathbf{F}_{\alpha\kappa} \cdot \mathbf{V}_\kappa \quad \alpha, \kappa = \beta, \gamma \quad \alpha \neq \kappa \end{aligned} \quad (70)$$

where the coefficients $\mathbf{F}_{\alpha\kappa}$ in the additional Forchheimer-like terms depends on the velocities. How? This is not well understood at this time, compared to the more thorough understanding available for the one-phase flow case (see above discussion). These models require to determine several effective properties which depend non-linearly upon saturation and velocities, which today is a challenging task not well understood.

To illustrate the capabilities of the various models, let us consider flow in a vertical column of high permeability (and hence low capillary effects) initially saturated by a liquid phase, β , and subjected to the upward flow of a gas phase, γ . Using the more general form Eq. 70, the case $\mathbf{V}_\beta = 0$ requires that

$$0 = -\frac{1}{\mu_\beta} K_\beta \left(\frac{\partial P_\beta}{\partial z} - \rho_\beta \mathbf{g} \cdot \mathbf{e}_z \right) + (K_{\beta\gamma} - F_{\beta\gamma}) V_\gamma \quad (71)$$

With the classical generalized Darcy's law, i.e., $(K_{\beta\gamma} - F_{\beta\gamma}) = 0$, the β -phase will drain until reaching the retention saturation which is very small in the case of a highly permeable medium. On the contrary, keeping the extra terms in Eq. 71 allows to account for liquid retention due to the drag force imposed on the liquid by the upward flow. This is true for the generalized model in Eqs. 70, for both Darcean and inertia regime. Models with drag forces like the one in Eqs. 68 and 69 have also the ingredients to account for the retention. The discussion would be on the expressions to be used. For instance [88] proposes a quadratic dependence while expressions like $(K_{\beta\gamma} - F_{\beta\gamma})$ offer a linear plus a quadratic term (with potentially even more complex dependence).

4.0 HEAT TRANSFER IN POROUS MEDIA PROBLEM

In this section, the major results corresponding to the classical heat transfer in porous media problem, i.e., diffusion/convection in the fluid saturating the pore space and conduction in the solid phase, are reviewed. This is a generic problem that embodies most of the individual features encountered in other transport mechanisms. For instance a zero solid conductivity would correspond to the problem of dispersion of a tracer. The exchange of heat between the phases is a typical example of double-porosity problem. Etc...

It is assumed that the flow is laminar and that the fluid density and viscosity are constant. As a consequence, the total mass balance problem and the momentum balance problem can be solved independently. In fact it suffices that the variations of density and viscosity over a representative unit cell are small. One must remember that this is a drastic assumption that may fail to be valid in the case of intense phase change, for instance. As a consequence of the above decoupling assumption, the macro-scale and micro-scale velocity fields are dealt with independently and are known fields for the pure heat transfer problem described by the following equations

$$(\rho c_p)_\beta \frac{\partial T_\beta}{\partial t} + (\rho c_p)_\beta \nabla \cdot (\mathbf{v}_\beta T_\beta) = \nabla \cdot (k_\beta \nabla T_\beta) \quad \text{in } V_\beta \quad (72)$$

$$T_\beta = T_\sigma \quad \text{at } A_{\beta\sigma} \quad (73)$$

$$\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla T_\sigma \quad \text{at } A_{\beta\sigma} \quad (74)$$

$$(\rho c_p)_\sigma \frac{\partial T_\sigma}{\partial t} = \nabla \cdot (k_\sigma \nabla T_\sigma) \quad \text{in } V_\sigma \quad (75)$$

where $(\rho c_p)_\alpha$, T_α , k_α are the α -phase specific heat, temperature and thermal conductivity respectively, and \mathbf{v}_β is the velocity field.

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This part objective is not to give the complete mathematical developments but rather to put the emphasis on the different modeling options that emerge, depending on the assumptions made. Therefore, only major steps that illustrate this discussion are reproduced here, using the framework of the theory of volume averaging ([19]) as a mere guideline. Additional literature will be cited to complete the learning process for those interested in the upscaling details.

4.1 The structure of the micro-macro coupled problem

As schematically described in Sec. 2.1, one needs to develop the coupled macro-scale and micro-scale equations. Only are listed below the averaged and deviation equation for the β -phase as well as the boundary conditions at $A_{\beta\sigma}$.

Averaging of Eq. 72 leads to

$$\begin{aligned}
 & \underbrace{\varepsilon_{\beta}(\rho c_p)_{\beta} \frac{\partial \langle T_{\beta} \rangle^{\beta}}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_{\beta}(\rho c_p)_{\beta} \langle \mathbf{v}_{\beta} \rangle^{\beta} \cdot \nabla \langle T_{\beta} \rangle^{\beta}}_{\text{convection}} = \\
 & \underbrace{\nabla \cdot \left[k_{\beta} \left(\varepsilon_{\beta} \nabla \langle T_{\beta} \rangle^{\beta} + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_{\beta} dA \right) \right]}_{\text{conduction/tortuosity}} \\
 & - \underbrace{(\rho c_p)_{\beta} \nabla \cdot \langle \tilde{\mathbf{v}}_{\beta} \tilde{T}_{\beta} \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla T_{\beta} dA}_{\text{interfacial flux}} \quad (76)
 \end{aligned}$$

where the traditional terms arising when upscaling flows in porous media, i.e., dispersion, tortuosity effects and exchange terms, have been emphasized. In this equation, the following decompositions of the pore-scale temperatures

$$T_{\alpha} = \langle T_{\alpha} \rangle^{\alpha} + \tilde{T}_{\alpha} \quad (77)$$

have been adopted.

The micro-scale equation is written as

$$\begin{aligned}
 & (\rho c_p)_{\beta} \frac{\partial \tilde{T}_{\beta}}{\partial t} + (\rho c_p)_{\beta} \tilde{\mathbf{v}}_{\beta} \cdot \nabla \langle T_{\beta} \rangle^{\beta} + (\rho c_p)_{\beta} \mathbf{v}_{\beta} \cdot \nabla \tilde{T}_{\beta} = \nabla \cdot (k_{\beta} \nabla \tilde{T}_{\beta}) \\
 & - \varepsilon_{\beta}^{-1} \nabla \cdot \left(k_{\beta} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_{\beta} dA \right) - \varepsilon_{\beta}^{-1} k_{\beta} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \nabla \tilde{T}_{\beta} dA \quad (78)
 \end{aligned}$$

Similar equations are developed for the σ -phase. The boundary conditions at $A_{\beta\sigma}$ are given by

$$\tilde{T}_{\beta} = \tilde{T}_{\sigma} - \underbrace{\left(\langle T_{\beta} \rangle^{\beta} - \langle T_{\sigma} \rangle^{\sigma} \right)}_{\text{source term}} \quad (79)$$

$$-\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla \tilde{T}_{\beta} - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla \langle T_{\beta} \rangle^{\beta}}_{\text{source term}} = -\mathbf{n}_{\beta\sigma} \cdot k_{\sigma} \nabla \tilde{T}_{\sigma} - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_{\sigma} \nabla \langle T_{\sigma} \rangle^{\sigma}}_{\text{source term}} \quad (80)$$

where the *source terms* that will trigger the development of temperature deviations have been emphasized.

4.2 Various models

This coupled problem for the two macro-scale equations and the two micro-scale equations is characterized by several time and length scales. Depending on the way these different scales are ordered, different approximations may be used leading to different macro-scale models. To make it short, let us consider the time-scales defined by the following estimates: $\frac{(\rho c_p)_\beta l_\beta^2}{k_\beta}$, $\frac{(\rho c_p)_\sigma l_\sigma^2}{k_\sigma}$, $\frac{\varepsilon_\beta (\rho c_p)_\beta L^2}{K_\beta^*}$ and $\frac{\varepsilon_\sigma (\rho c_p)_\sigma L^2}{K_\sigma^*}$, where the characteristic macro-scale diffusivities K_β^* and K_σ^* will be specified a posteriori.

4.2.1 Local equilibrium

Local equilibrium arises when all length-scales are well separated between the macro-scale and the micro-scale and when the pore-scale characteristic times are similar. In particular, one has

$$\left(\frac{(\rho c_p)_\beta l_\beta^2}{k_\beta} \approx \frac{(\rho c_p)_\sigma l_\sigma^2}{k_\sigma} \right) \ll \left(\frac{\varepsilon_\beta (\rho c_p)_\beta L^2}{K_\beta^*} \approx \frac{\varepsilon_\sigma (\rho c_p)_\sigma L^2}{K_\sigma^*} \right) \quad (81)$$

As a consequence, the two macro-scale temperatures are close enough so one can introduce the approximation

$$\langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T \rangle \quad (82)$$

with the total heat for the mixture given by

$$\varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \varepsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma = (\rho c_p)^* \langle T \rangle \quad (83)$$

in which the effective heat capacity is a simple average: $(\rho c_p)^* = \varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma$. Under these circumstances, one may derive a simple closure with the following estimates for the temperature deviations ([99])

$$\tilde{T}_\beta = \mathbf{b}_\beta(\mathbf{y}) \cdot \nabla \langle T \rangle(\mathbf{x}, t) + \dots \quad (84a)$$

$$\tilde{T}_\sigma = \mathbf{b}_\sigma(\mathbf{y}) \cdot \nabla \langle T \rangle(\mathbf{x}, t) + \dots \quad (84b)$$

The mapping vectors, \mathbf{b}_β and \mathbf{b}_σ , are given by a steady-state closure problem expressed as

$$(\rho c_p)_\beta \tilde{\mathbf{v}}_\beta + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{b}_\beta = k_\beta \nabla^2 \mathbf{b}_\beta \text{ in } V_\beta \quad (85a)$$

$$\text{B.C.1} \quad -\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \mathbf{b}_\beta - \mathbf{n}_{\beta\sigma} k_\beta = -\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \mathbf{b}_\sigma - \mathbf{n}_{\beta\sigma} k_\sigma \text{ at } A_{\beta\sigma} \quad (85b)$$

$$\text{B.C.2} \quad \mathbf{b}_\beta = \mathbf{b}_\sigma \text{ at } A_{\beta\sigma} \quad (85c)$$

$$0 = k_\sigma \nabla^2 \mathbf{b}_\sigma \text{ in } V_\sigma \quad (85d)$$

$$\mathbf{b}_\beta(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_\beta(\mathbf{x}) ; \mathbf{b}_\sigma(\mathbf{x} + \mathbf{l}_i) = \mathbf{b}_\sigma(\mathbf{x}) \quad i = 1, 2, 3 \quad (85e)$$

$$\langle \mathbf{b}_\beta + \mathbf{b}_\sigma \rangle = 0 \quad (85f)$$

Adding Eq. 78 with its σ -phase counterpart, and substituting the deviations by their expressions Eqs. 84, one obtains the following macro-scale equation

$$(\rho c_p)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \mathbf{U}_\beta \cdot \nabla \langle T \rangle = \nabla \cdot (\mathbf{K}_{eq}^* \cdot \nabla \langle T \rangle) \quad (86)$$

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where the effective thermal conductivity tensor is given by

$$\mathbf{K}_{eq}^* = (\varepsilon_\beta k_\beta + \varepsilon_\sigma k_\sigma) \mathbf{I} + \frac{k_\beta - k_\sigma}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_\beta dA - (\rho c_p)_\beta \langle \tilde{\mathbf{v}}_\beta \mathbf{b}_\beta \rangle^\beta \quad (87)$$

and where $\mathbf{U}_\beta = \langle \mathbf{v}_\beta \rangle^\beta$. This expression contains three contributions:

- a simple average of the thermal conductivity,
- a correction to this simple average due to the topology (tortuosity) of the phase repartition,
- a contribution that comes from the product of velocity and temperature deviations and which corresponds to the dispersion mechanisms.

Effective Thermal Conductivity

Let us discuss some properties of the first two terms which gives the effective thermal diffusion tensor. The existence of bounds has been already introduced in Sec. 2.0. This is illustrated in Fig. 4 for the classical Wiener's bounds. The figure shows that Wiener's bounds ([100]), as expressed by Eq. 19, are in general too far apart and more narrow bounds can be developed for *specific classes* of material, see a popular example in [101] or a more thorough discussion in [102]. They can be used to control experimental or theoretical determination of the effective thermal conductivity as well as "semi-predictive" tools. The effective thermal conductivity can also be estimated experimentally or calculated by solving Eqs. 85 over a representative unit cell of the porous medium, a strategy that becomes more and more popular with the development of CT-scanners or other devices for pore-scale investigation. Several correlations have been proposed in the literature, see some examples in [103–105]. The effective diffusivity is very sensitive to the topology and pore-scale physical characteristics, especially when the solid thermal conductivity is much larger than the fluid conductivity (about two order of magnitude) and when contacts exist between the solid inclusions ([106–108]). This behavior is illustrated in Fig. 5 taken from [109]. The figure represents the effective thermal diffusion divided by the β -phase thermal conductivity versus the ratio $\frac{k_\sigma}{k_\beta}$ for a given β -phase volume fraction and various geometries. Typically, one observes a plateau for high values of $\frac{k_\sigma}{k_\beta}$ in the case of non-touching particles. The behavior is the same for touching particles for moderate thermal conductivity ratios. However, the flux through the contact areas becomes very important at high values of $\frac{k_\sigma}{k_\beta}$, which leads to a continuous increase of the effective thermal conductivity. It must be understood that the resulting effective thermal conductivity is very sensitive to the contact area, itself highly dependent on various mechanisms: manufacturing, stress, ...

Effective thermal dispersion

Dispersion mechanisms, as shown by the third term in Eq. 87, depend on the statistical properties of the product of the velocity fluctuations by the temperature fluctuations. If one puts $k_\sigma = 0$ in the closure problem, one recovers the traditional dispersion tensor corresponding to the dispersion equation for a tracer of averaged concentration $\langle c_\beta \rangle^\beta$. The dispersion equation reads

$$\frac{\partial \varepsilon_\beta \langle c_\beta \rangle^\beta}{\partial t} + \nabla \cdot (\varepsilon_\beta \langle c_\beta \rangle^\beta \mathbf{U}_\beta) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_\beta^* \cdot \nabla \langle c_\beta \rangle^\beta) \quad (88)$$

where \mathbf{D}_β^* is the dispersion tensor. For a uniform macro-scale flow aligned with the x -axis, the longitudinal dispersion coefficient has the behavior illustrated in Fig. 6 as a function of the pore-scale Péclet number defined as

$$Pe = \frac{U_\beta d_p}{D_\beta} \quad (89)$$

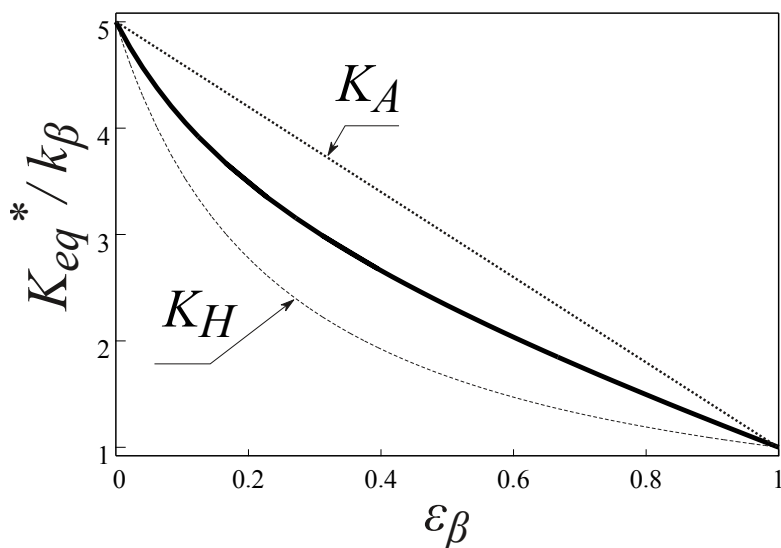


Figure 4: Illustration of classical bounds for the effective thermal conductivity (curves for a given value of the thermal conductivity ratio).

where D_β is the molecular diffusion coefficient. One distinguishes in Fig. 6 a diffusive regime for small Péclet numbers followed, after some transition, by a dispersion regime characterized by $D_{\beta xx}^* \sim Pe^n$. The exponent is equal to 2 in the case of Taylor's dispersion (dispersion in a tube subjected to a Poiseuille flow, [110]), nearly equal to 2 for simple unit cells and tends towards a linear regime i.e., $n=1$, for highly disordered porous media. The power law regime does not hold beyond a certain value of the Péclet number for the experimental data. The reader is referred to the discussion in [19] for an explanation of this result. Another important characteristic of dispersion is the highly anisotropic feature of the tensor due to the flow. This is illustrated in Fig. 7, which represents the longitudinal, D_L , versus the transversal, D_T , dispersion coefficient, as defined with respect to the flow direction. In the diffusive regime, the two values are equal if the medium is geometrically isotropic, while in the fully developed dispersion regime their value are in the ratio of one order of magnitude.

The fundamental characteristics of the pure dispersion case are reflected in the case of thermal dispersion. However, the results are more complicated due to the transfer to the solid phase. This is illustrated in Fig. 8 from [111], which shows the ratio of the longitudinal thermal dispersion coefficient divided by the thermal conductivity of the liquid phase versus the Péclet number. One sees indeed a diffusive regime followed by a dispersion regime. However, due to transfer through the solid phase, values are different. In particular, the transition regime appears for larger Péclet numbers.

4.2.2 Non-equilibrium models

Non-equilibrium models arise when the transport properties of the various phases are highly contrasted. For instance, the diffusivity of the solid phase is much lower than the diffusivity of the fluid phase. In this case, the heat wave goes rapidly through the unit cell in the liquid phase and the temperature field relaxes slowly in the solid phase, thus producing a well-known tailing effect. The relaxation process involves many different time-scales (the spectrum is controlled by the eigenvalues of the diffusion problem over the solid phase). This makes the solution of the coupled problem described in Sec. 4.1 non-local in time (memory effects), and perhaps in space (i.e., the solution depends on all time and space values). Indeed, a closure keeping all local time-scales

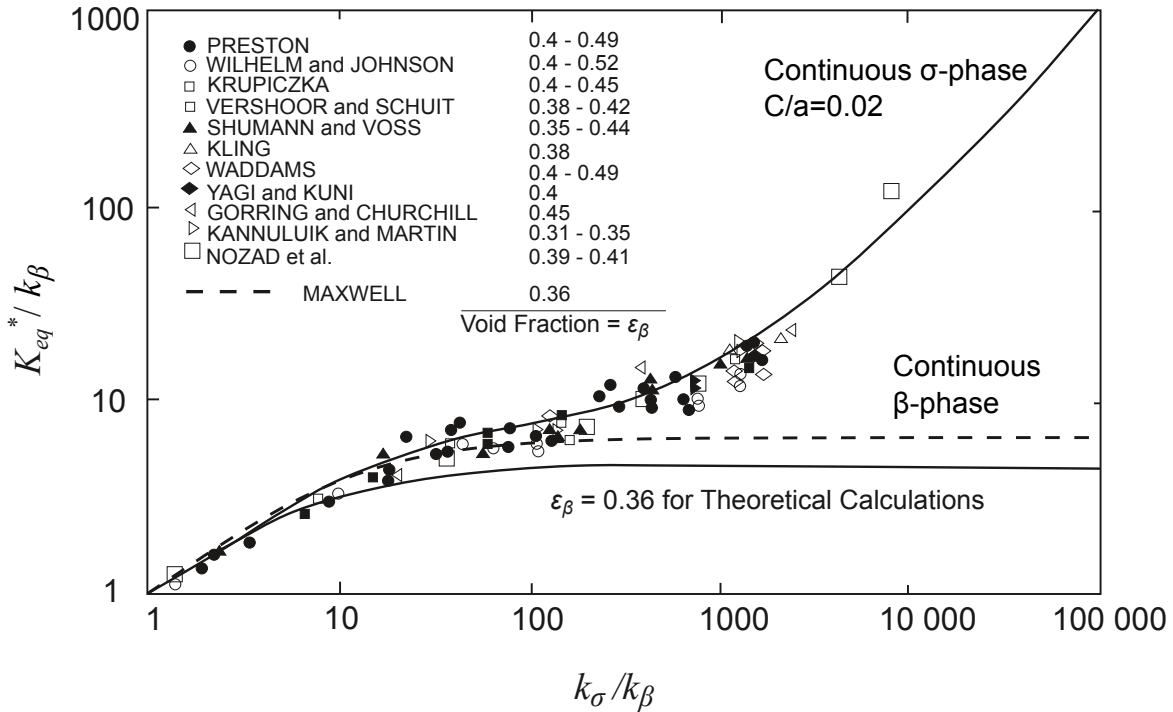


Figure 5: Contact point effects for the effective thermal conductivity (after [109]).

involves a time convolution as has been discussed in [112] for a pure conductive problem and in [113] from a more general perspective. The deviations in this case are expressed as

$$\tilde{T}_\beta = \mathbf{b}_{\beta\beta} \star \frac{\partial}{\partial t} \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_\sigma \rangle^\sigma - s_\beta \star \frac{\partial}{\partial t} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \dots \quad (90a)$$

$$\tilde{T}_\sigma = \mathbf{b}_{\sigma\beta} \star \frac{\partial}{\partial t} \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_\sigma \rangle^\sigma + s_\sigma \star \frac{\partial}{\partial t} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \dots \quad (90b)$$

where the mapping variables closure problems are time-dependent. The mapping variables relax more rapidly towards an asymptotic value with time than the macro-scale temperatures and one may seek a steady-state closure under the following form ([99, 111, 114–116])

$$\tilde{T}_\beta = \mathbf{b}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma - s_\beta \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + \dots \quad (91a)$$

$$\tilde{T}_\sigma = \mathbf{b}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + s_\sigma \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + \dots \quad (91b)$$

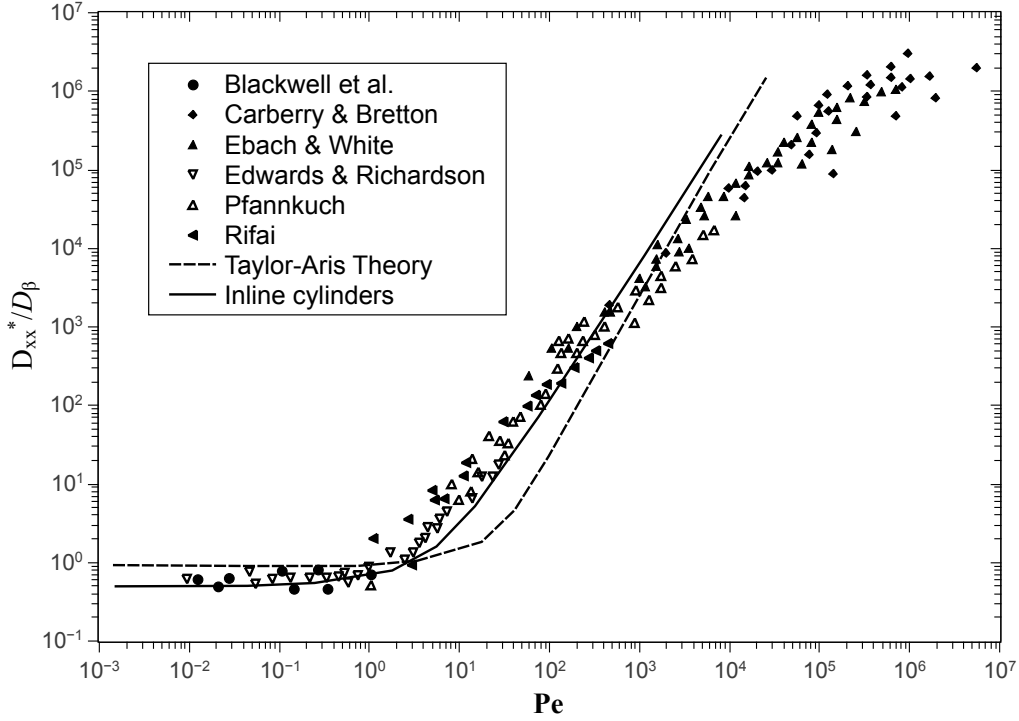


Figure 6: Logitudinal Dispersion Coefficient (after [19]).

where the mapping variables are the limit of the time dependent closure for $t \rightarrow \infty$. As an example, the problem for the mapping variables s_β and s_σ is given by

$$(\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla s_\beta = k_\beta \nabla^2 s_\beta - \varepsilon_\beta^{-1} h_\beta \quad , \text{ in } V_\beta \quad (92a)$$

$$\text{B.C.1. } \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla s_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla s_\sigma \quad , \text{ at } A_{\beta\sigma} \quad (92b)$$

$$\text{B.C.2. } s_\beta = 1 + s_\sigma \quad , \text{ at } A_{\beta\sigma} \quad (92c)$$

$$0 = k_\sigma \nabla^2 s_\sigma + \varepsilon_\sigma^{-1} h_\sigma \quad , \text{ in } V_\sigma \quad (92d)$$

$$s_\beta(\mathbf{r} + \mathbf{l}_i) = s_\beta(\mathbf{r}), \quad s_\sigma(\mathbf{r} + \mathbf{l}_i) = s_\sigma(\mathbf{r}) \quad , \quad i = 1, 2, 3 \quad (92e)$$

$$\langle s_\beta \rangle = 0 \quad ; \quad \langle s_\sigma \rangle = 0 \quad (92f)$$

$$h_\beta = \langle \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla s_\beta \delta_{\beta\sigma} \rangle \quad ; \quad h_\sigma = -\langle \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla s_\sigma \delta_{\beta\sigma} \rangle = h_\beta = h_{2eq} \quad (92g)$$

where $\delta_{\beta\sigma}$ is the surface Dirac function on $A_{\beta\sigma}$. It is of a fundamental importance to see that the heat exchange coefficient, h_{2eq} , is a result of this integro-differential closure problem and not given a priori. Using this steady-state closure, the macro-scale equations can be written under the form of a generalized two-equation model as

$$\begin{aligned} \varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \\ \nabla \cdot \left(\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) \end{aligned} \quad (93a)$$

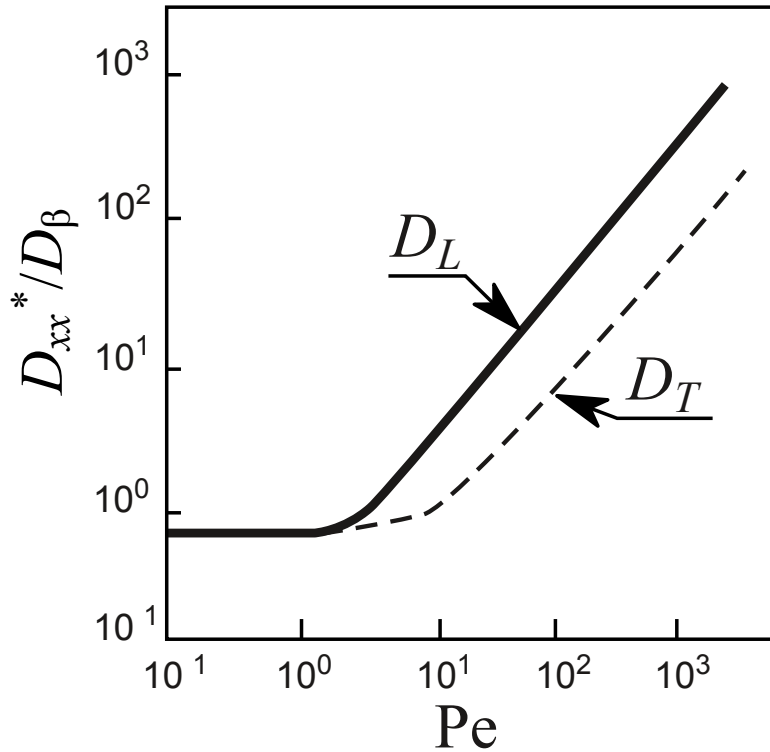


Figure 7: Longitudinal Dispersion Coefficient versus Transversal Dispersion Coefficient.

$$\varepsilon_{\sigma} (\rho c_p)_{\sigma} \frac{\partial \langle T_{\sigma} \rangle^{\sigma}}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_{\beta} \rangle^{\beta} - \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_{\sigma} \rangle^{\sigma} = \nabla \cdot \left(\mathbf{K}_{\sigma\beta}^* \cdot \nabla \langle T_{\beta} \rangle^{\beta} + \mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_{\sigma} \rangle^{\sigma} \right) - h_{2eq} \left(\langle T_{\sigma} \rangle^{\sigma} - \langle T_{\beta} \rangle^{\beta} \right) \quad (93b)$$

where the various effective parameters are obtained from the mapping variables. Making $\langle T_{\beta} \rangle = \langle T_{\sigma} \rangle$, one recovers the one equation equilibrium model with

$$\mathbf{K}_{eq}^* = \mathbf{K}_{\beta\beta}^* + \mathbf{K}_{\beta\sigma}^* + \mathbf{K}_{\sigma\beta}^* + \mathbf{K}_{\sigma\sigma}^* \quad (94)$$

Before discussing some properties of the effective parameters, one must note that simpler closures may be used depending on the assumptions made on the physical characteristics of the problem ([23, 117]). Similarly, if one drops the additional convective and cross-terms¹, one recover the traditional two-equation model often used in the literature ([119, 120]).

The two phase effective thermal dispersion tensors are often estimated as

$$K_{\beta\beta}^* = \varepsilon_{\beta} k_{\beta} \quad ; \quad K_{\beta\sigma}^* = K_{\sigma\beta}^* = 0 \quad ; \quad K_{\sigma\sigma}^* = \varepsilon_{\sigma} k_{\sigma} \quad (95)$$

¹The reader must be warned that these additional terms may play a role if one wants to have an accurate theory, as is illustrated in [118]

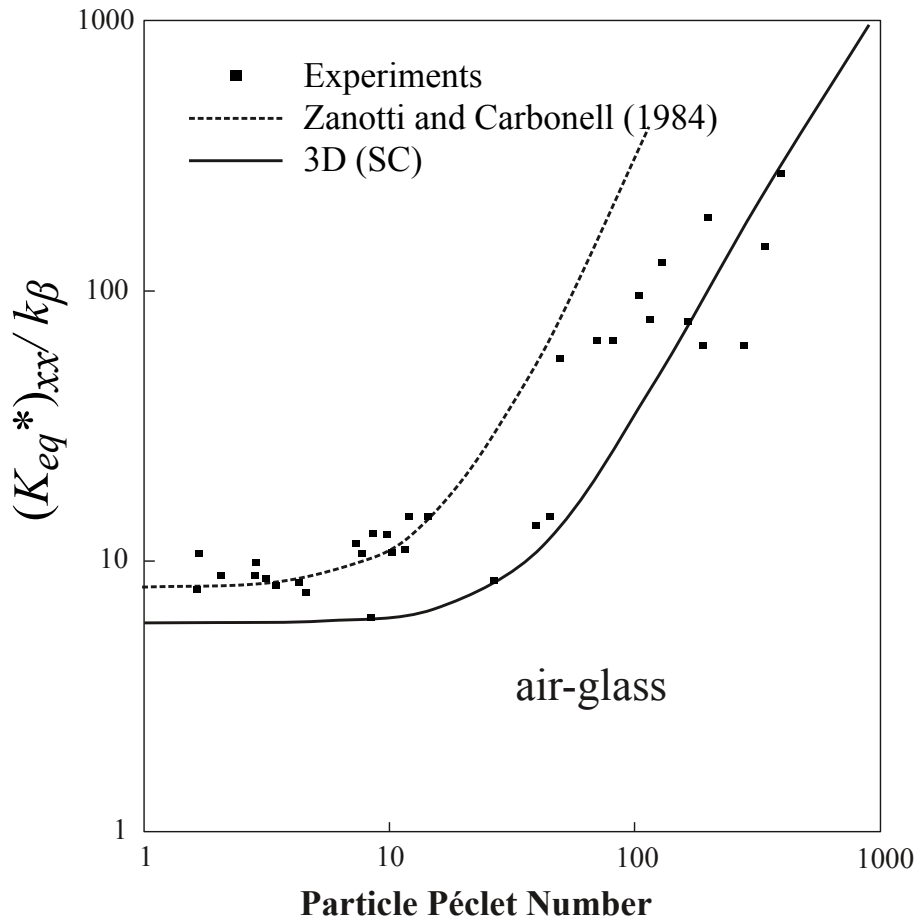


Figure 8: Effective longitudinal thermal dispersion coefficient for an Air-Glass system.

which in turn implies from Eq. 96 that

$$K_{eq}^* = \varepsilon_{\beta} k_{\beta} + \varepsilon_{\sigma} k_{\sigma} \tag{96}$$

i.e., a simple arithmetic average of the pore-scale values, which is in general a bad estimate as discussed in Sec. 4.2.1. Therefore, values in Eqs. 95 must be used with care. One can consult [111] for the calculation of the various tensors from a pore-scale geometry, as well as some discussion of the impact of the Péclet number and the thermal conductivity ratio.

The heat exchange coefficient, h_{2eq} , corresponds to a single relaxation time as opposed to the full spectrum discussed in the introduction to this section. Hence, this is not exactly an intrinsic property of the porous medium and its value depends on the theory used to define it or the measurement method, for instance the objective function if using an inverse method. This explains why several values have been proposed in the literature as discussed in [121] in the case of pure diffusion in a system with a lower diffusivity in the solid. In this case, the proposed values are related to the eigenvalue spectrum of the solid grain diffusive problem in different ways, for instance the first eigenvalue, etc.... The value obtained from the closure problem described by Eqs. 92 plays a fundamental role, as will be shown in Sec. 4.2.2, and is related to the harmonic mean of the eigenvalues.

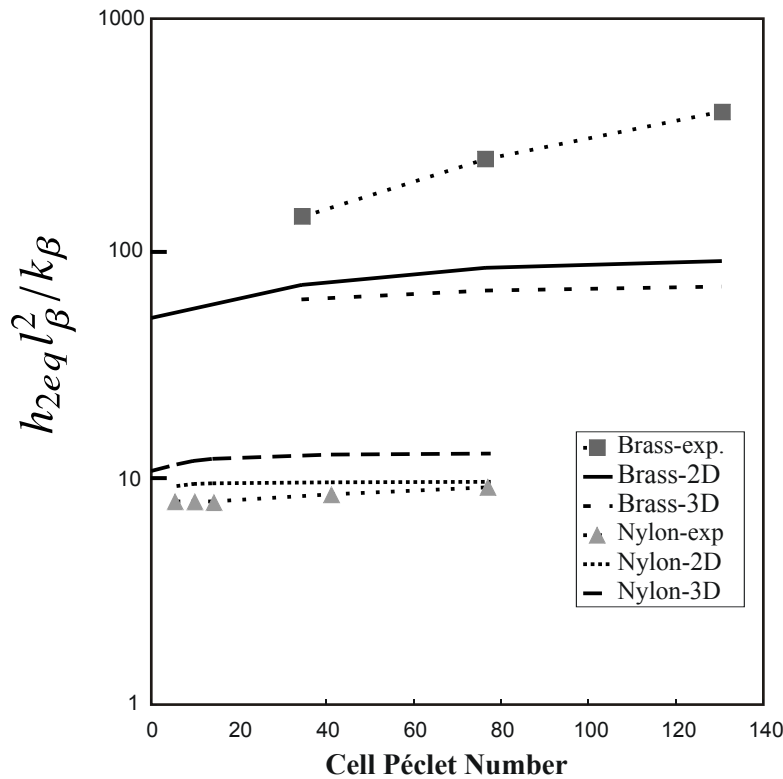


Figure 9: Theoretical and experimental values of the exchange coefficient as a function of the Péclet number for two sets of phases (adapted from [111])

Another problem comes from the periodicity conditions which are often used when solving closure problems (as is the case in Eq. 92e). If one takes, as an analogy of a porous medium problem, heat transfer in a tube (ie, e Graetz problem), such conditions are in fact compatible with the established regime ([118]). This produces a smaller impact of the pore-scale Péclet number on the effective heat exchange coefficient as one would estimate by taking into account *entrance* effects. Such effects would lead to a non-local (in space) analysis, i.e., local transport parameters would depend on the distance from the inlet boundary. They also contribute to the differences encountered in the literature between the different correlations or estimates of the heat exchange coefficient.

An example of calculation of the heat exchange coefficient is illustrated in Fig. 9. The experimental and theoretical values are in good agreement for the nylon-water system characterized by a low thermal conductivity ratio, while the agreement is not as good for a higher conductivity ratio, which suggests some contact point effects, as discussed above. The heat exchange coefficient is also often written as

$$h_{2eq} = a_v h \quad (97)$$

where $a_v = \frac{A_{\beta\sigma}}{V}$ is the porous medium specific surface and h is an *intrinsic* heat transfer coefficient. This comes from the *supposed* existence of an established film or boundary layer at the pore-scale that can be introduced as a pore-scale boundary condition at $A_{\beta\sigma}$. Indeed, assuming that such a boundary condition exists at the pore-scale, one recovers from the upscaling process a two-equation model with an exchange term written like Eq. 97 ([122, 123]). However, it is clear that h should be a result of the upscaling development and not an input. Furthermore, while the appearance of a_v is natural in some upscaling processes, equilibrium adsorption

for instance, this is not the case here since the problem giving h_{2eq} , Eqs. 92a through 92g, involves a diffusive process which will generate cut-off or smoothing effects for rough or fractal surfaces. Therefore, Eq. 97 is not true in general. This problem is often overlooked in the literature.

The problem of the conditions for the existence of two-temperature regimes has received a lot of attention in the literature ([116, 124–128]). Simple estimates of the various time and length-scales may often be enough in many practical instances to decide whether a non-equilibrium analysis is needed or not, if differences are clear (for instance several order of magnitude). If this is not the case, the matter is more complex and this depends on the geometry and topology of the unit cell ([116]), the boundary value problem solved ([128, 129]), the processes involved, e.g. natural convection ([130]), phase change ([131, 132]), the coupling with reactive transport ([133, 134]), etc...

Asymptotic behavior and One-Equation Non-Equilibrium model

It has been shown in [113–115] that the two equation model can be approximated asymptotically as $t \rightarrow \infty$ for a uniform 1D flow in a semi-infinite or infinite domain by a classical heat equation

$$\left(\epsilon_{\beta} (\rho c_p)_{\beta} + \epsilon_{\sigma} (\rho c_p)_{\sigma} \right) \frac{\partial \langle T \rangle^{\beta\sigma}}{\partial t} + \epsilon_{\beta} (\rho c_p)_{\beta} \langle \mathbf{v}_{\beta} \rangle^{\beta} \cdot \nabla \langle T \rangle^{\beta\sigma} = \nabla \cdot \left(\mathbf{K}_{\infty}^* \cdot \nabla \langle T \rangle^{\beta\sigma} \right) \quad (98)$$

where

$$\langle T \rangle^{\beta\sigma} = \frac{\left(\epsilon_{\beta} (\rho c_p)_{\beta} \langle T_{\beta} \rangle^{\beta} + \epsilon_{\sigma} (\rho c_p)_{\sigma} \langle T_{\sigma} \rangle^{\sigma} \right)}{\left(\epsilon_{\beta} (\rho c_p)_{\beta} + \epsilon_{\sigma} (\rho c_p)_{\sigma} \right)} \quad (99)$$

is the mixture average temperature and in which \mathbf{K}_{∞}^* is given by (dropping cross terms)

$$\mathbf{K}_{\infty}^* = \mathbf{K}_{eq}^* + \frac{1}{h_{2eq}} \frac{\left(\epsilon_{\beta} (\rho c_p)_{\beta} \epsilon_{\sigma} (\rho c_p)_{\sigma} \right)^2}{\left(\epsilon_{\beta} (\rho c_p)_{\beta} + \epsilon_{\sigma} (\rho c_p)_{\sigma} \right)^2} \mathbf{U}_{\beta} \mathbf{U}_{\beta} \quad (100)$$

One sees from this equation that the effective asymptotic thermal dispersion tensor is obviously greater than the local equilibrium value, \mathbf{K}_{eq}^* . One must emphasize that the one-equation non-equilibrium model does not imply that the two-averaged temperature are equal. This merely means that the front spreading masks asymptotically the lag between the two average temperatures, as discussed in [113, 115]. Another important discovery is that a direct closure can be found based on $\langle T \rangle^{\beta\sigma}$ ([45, 135, 136]) if one looks at the pore-scale temperature fields through the following decomposition

$$\hat{T}_{\beta} = T_{\beta} - \langle T \rangle^{\beta\sigma} \approx \mathbf{b}_{\beta}^{\infty} \cdot \nabla \langle T \rangle^{\beta\sigma} ; \hat{T}_{\sigma} = T_{\sigma} - \langle T \rangle^{\beta\sigma} \approx \mathbf{b}_{\sigma}^{\infty} \cdot \nabla \langle T \rangle^{\beta\sigma} \quad (101)$$

It was proven numerically and analytically ([45, 136]) that the resulting non-equilibrium one-equation model is similar to Eq. 98 and that the two effective thermal dispersion tensors (two-equation asymptotic behaviour and one-equation non-equilibrium closure) are equal *if* the heat exchange coefficient is the one from the closure provided by Eqs. (92). To be clear enough, the use of other estimates (see [121]) may lead to erroneous effective thermal conductivity.

Other non-equilibrium one-equation models have been proposed in the literature. For instance, it has been shown in [137] that the two-equation model is equivalent under certain conditions to a dual-phase-lagging heat conduction model. Similarly, it must be noticed that other types of equations may potentially reproduce some of the features of local non-equilibrium situations, for instance equations with fractional derivatives which have already been used for dealing with some problems of dispersion in porous media ([138]).

Introduction to Heat and Mass Transport in Porous Media

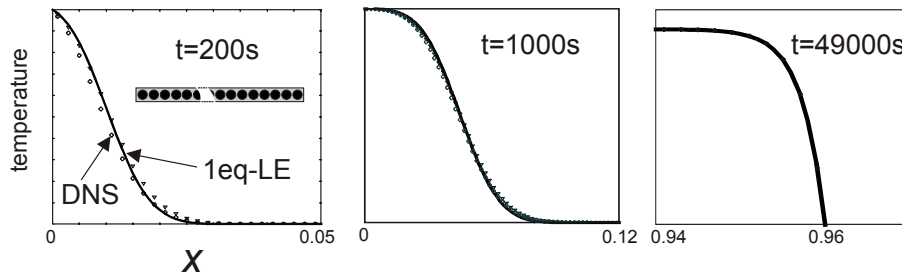


Figure 10: Transient evolution of macro-scale models (adapted from [139])

Discussion

At this point, one has already at hand several models for the *same* initial pore-scale problem! The reader is referred to [136] (see in particular Fig. 8) for an exploration of their domain of validity for a typical boundary value problem. It is also of a fundamental importance to recognize that transitions between these various models may arise for the same Initial Boundary Value Problem as has been shown in [139] (this problem is also revisited in [7]). Fig. 10 represents the averaged temperature fields obtained from direct pore-scale numerical simulations (symbols) over an array of cylinders (injection from the left at constant temperature, Dirichlet condition at the exit) and the one-equation local equilibrium solution. One sees that:

- at early stages (graph on the left) the solution calls for a local non-equilibrium treatment,
- the asymptotic behavior is later observed (middle graph), characterized by a larger thermal conductivity (larger spreading of the thermal plume) than the one-equation equilibrium model,
- because of the boundary condition at the exit, the *conditions revert to local equilibrium* (graph on the right)! An error would be made if one would attempt to predict this final temperature field with the asymptotic thermal conductivity value.

From this discussion and the proposed example, one has to be careful when recommending the exclusive use of such and such model, as is sometimes the case in the literature. The suggested model may be acceptable during a time interval and may fail after. This is particular true for the asymptotic model since specific conditions are needed to reach the asymptotic limit. Any event that would recondition the temperature fields may lead to its failure. It must be acknowledged that, while it cannot recover all the characteristic times involved in a given thermal process, the two-equation model has the ability to reproduce several regimes since it also includes the asymptotic model and the local equilibrium model. This robustness may be used to assess, at the expense of some limited additional complexity, whether the particular process of interest may be affected by local non-equilibrium effects or not.

The limitations of the two-equation model with a single linear or first-order exchange term, i.e., with a single characteristic time for describing the fluid-solid temperature relaxation, have already been indicated. This inaccuracy may in principle be overcome through the use of the full model with convolution products. However, convolution products are not handy for numerical implementations. Alternate models have been designed to incorporate more characteristic times in the macro-scale equations. One class of models is called multi-rate models, see [140] for an introduction. In general, they may be derived by a splitting of the temperature fields into several sub-phases, either defined by geometrical considerations (for instance grains of big diameters and grains of small diameters) or through a more sophisticated mathematical point of view, for instance using the

properties of the eigenvalue spectrum for the diffusion process into the solid phase. This in general leads to N-equation models, which may reproduce the expected several characteristic time behavior without the inconvenience of using convolution products.

A final class of model, called mixed or hybrid models, is based on the following approximation: if the solid phase thermal diffusivity is two order of magnitude, or more, smaller than the fluid thermal conductivity, i.e., $k_\sigma \sim \epsilon^2 k_\beta$, then Eq. (80) may be approximated by

$$\langle T_\beta \rangle^\beta + \underbrace{\tilde{T}_\beta}_{O(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta)} = T_\sigma \quad \Rightarrow \quad \underbrace{\langle T_\beta \rangle^\beta}_{macro-scale} = \underbrace{T_\sigma}_{micro-scale} \quad (102)$$

The final model combines a micro-scale diffusion equation coupled through Eq. (102) to a macro-scale equation in which the effective thermal dispersion tensor is the one provided by Eqs. (85) with $k_\sigma = 0$. The mixed model works better than the two-equation model in that case, however, it does not work as well as the two-equation model for $k_\sigma \sim \epsilon k_\beta$, as emphasized in [141]. Another type of mixed model may be introduced when sharp thermal fronts are encountered as in [142] in the case of combustion in porous media: they correspond to the use of a micro-scale model in the front matched far from the front with a macro-scale model.

Finally, Fig. 11 summarizes schematically the various models that can be used: direct pore-scale numerical simulation, the various one-equation, 2-equation and N-equation models, as well as mixed models.

5.0 EXTENSIONS

In this section, some indications are provided about the extension of the previous models to several classes of problems of general practical importance.

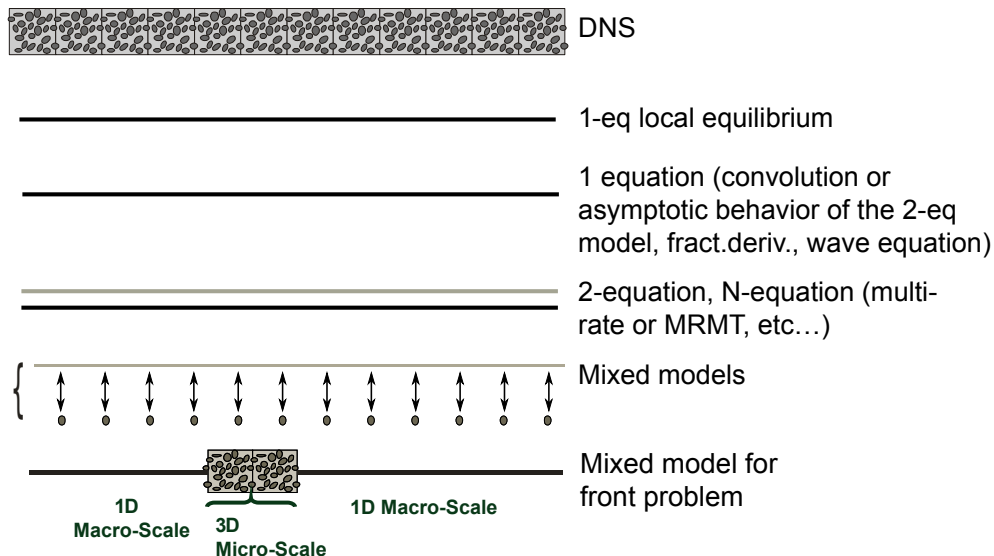


Figure 11: Multiple-scale description of a porous medium: various model-types.

5.1 Heterogeneous and homogeneous heat sources

Homogeneous or heterogeneous heat sources in the energy equations may be uncoupled to heat transfer, for instance in the case of the cooling of nuclear reactor debris beds where the heat source is produced by radioactivity, or may lead to strongly non-linear coupled problems, for instance in the case of smoldering or combustion in porous media. The uncoupled problem has been studied in [143] from an upscaling point of view. The case of local equilibrium can be treated in a very straightforward manner in the case of constant source terms. A constant homogeneous source term, for instance Φ_σ in the σ -phase, does not pose a problem and is simply added as $\varepsilon_\sigma \Phi_\sigma$ to the macro-scale relevant equation in the one-equation or two-equation model. The effect of the heterogeneous source, Ω , is more complicated and requires an additional closure problem that allows for the distribution of the heat source between the two equations, i.e., the two-temperature model becomes

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + a_v \xi \Omega \quad (103a)$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left(\mathbf{K}_{\sigma\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left(\langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + a_v (1 - \xi) \Omega + \varepsilon_\sigma \Phi_\sigma \quad (103b)$$

where ξ is a so-called *distribution coefficient* which can be calculated from the resolution of a fourth closure problem.

Numerical calculations of the distribution coefficient in [7, 143] shows that $\xi \rightarrow 0$ when $k_\sigma/k_\beta \rightarrow \infty$ which leads to the heuristic equation in which all the produced heat is affected to the solid phase ([134]). This behavior of the distribution coefficient is illustrated in Fig. 13. The figures report values for the two unit cells described in Fig. 12: a simple stratified unit cell for which the closure problem may be solved analytically, and a tomographic image of an unconsolidated medium, and for a simple 3D unit cell corresponding to a centered cubic array of spheres (legend "CC", FVM standing for Finite Volume Model). The results show the asymptotic behavior described above. The graphs for the two media are relatively different, thus suggesting a significant impact of the pore-scale geometrical features. It is interesting to note that this framework has been used to develop a local non-equilibrium model taking into account radiation effects through a generalized radiation transfer equation providing Ω in a coupled manner ([144]).

5.2 Reactive transport

The coupling with mass transfer and reaction is often treated with some sort of decoupling ([133, 134, 145]). Indeed, if one assumes that the mass reaction rate is of the form

$$r_\beta = F(c_\beta, T_\beta) = F\left(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta\right) + \frac{\partial F}{\partial c_\beta} \left(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta\right) \tilde{c}_\beta + \frac{\partial F}{\partial T_\beta} \left(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta\right) \tilde{T}_\beta + \dots \quad (104)$$

then neglecting deviation terms based on the estimate $\tilde{T}_\beta = \mathcal{O}\left(\frac{l_\beta}{L} \langle T_\beta \rangle^\beta\right)$ leads to

$$r_\beta = F(c_\beta, T_\beta) = F\left(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta\right) \quad (105)$$

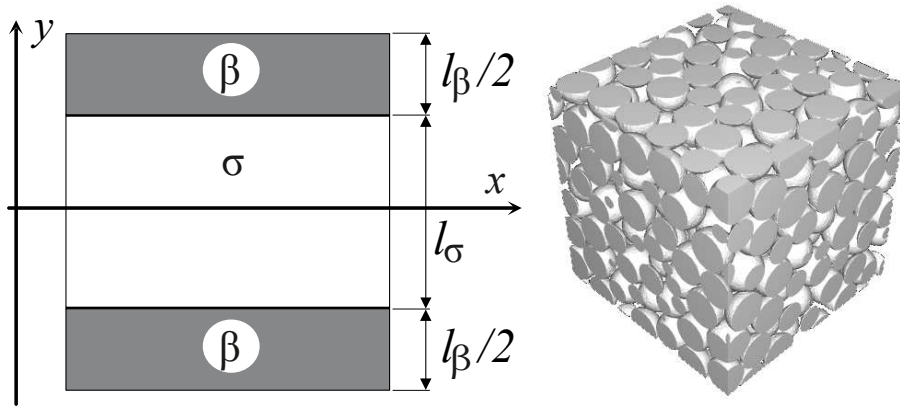


Figure 12: Unit Cell: stratified (left), data from X-ray Tomography (right).

As a consequence, the development remains the same as before but for the fact that the source term is treated as locally constant at a value $F(\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta)$. One understands that highly non-linear reaction terms, such as Arrhenius equations, or the potential existence of sharp combustion fronts may require more complicated closures ([133]) or even call for direct numerical simulations or mixed models ([142]). From an upscaling point of view, these problems remain largely open problems.

5.3 Coupling with momentum and mass transport

So far, the heat equation upscaling problem has been treated independently of the mass and momentum transport. This required neglecting density and viscosity variations. As emphasized above, coupling between the various transport problems may have to be considered. While this classification is not essential, one may distinguish weak and strong couplings, calling for very different upscaling techniques.

5.3.1 Weak couplings

Often, *weak coupling* can be treated following the ideas leading to Eq. (105), i.e., density, viscosity, thermal diffusion or mass diffusion are supposed to be constant (to make it simple) over the averaging volume at the intrinsic averaged temperature, pressure, concentration, etc. As a consequence, the closure problems have these averaged values as parameters and the resulting effective parameters will depend non-linearly on $\langle c_\beta \rangle^\beta, \langle T_\beta \rangle^\beta$.

Another class of coupled problems may be treated relatively easily: *one-sided coupling*. This is the case, for instance, when dealing with thermodiffusion and when Soret effect is only taken into account. Assuming constant fluid and solid characteristics, the thermal upscaling problem may be treated independently of the species transport problem which is defined by

$$\frac{\partial c_\beta}{\partial t} + \nabla \cdot (c_\beta \mathbf{v}_\beta) = \nabla \cdot (D_\beta \nabla c_\beta + D_{T\beta} \nabla T_\beta) \quad (106)$$

$$\text{B.C.1} \quad \mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla c_\beta + D_{T\beta} \nabla T_\beta) = 0 \quad \text{at } A_{\beta\sigma} \quad (107)$$

Because of this one-side coupling, the temperature deviations can be estimated from the various closures presented in this paper, i.e., Eqs. (84) or (91). In turn, it can be introduced in the mapping expression for the

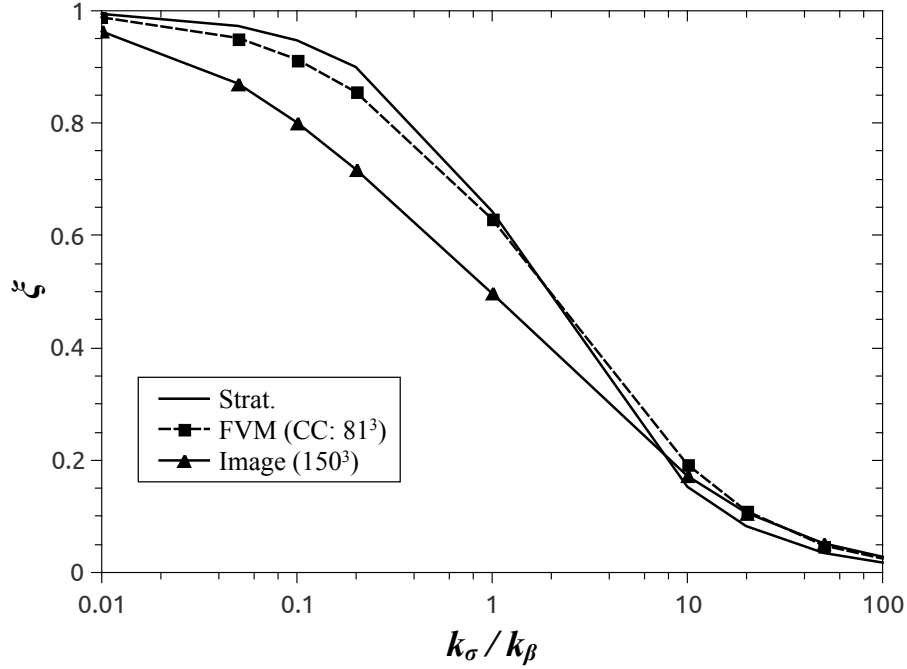


Figure 13: Values of the distribution coefficient as a function of the thermal conductivity ratio for three types of media: a stratified unit cell, a cubic centered array of spheres, a CT-Scan image of an unconsolidated medium (N^3 refers to the number of voxels describing the medium).

concentration deviation. For instance, the local equilibrium closure would lead to ([139])

$$\tilde{c}_\beta = \mathbf{b}_{C\beta} \cdot \nabla \langle c_\beta \rangle^\beta + \mathbf{b}_{S\beta} \cdot \nabla \langle T \rangle \quad (108)$$

The closure problems for $\mathbf{b}_{C\beta}$ is the classical problem leading to the dispersion tensor ([53, 146]) while the closure problem for $\mathbf{b}_{S\beta}$ is coupled with the closure problem for \mathbf{b}_β described by Eqs. (85). One has

$$\mathbf{v}_\beta \cdot \nabla \mathbf{b}_{S\beta} = D_\beta \nabla^2 \mathbf{b}_{S\beta} + D_{T\beta} \nabla^2 \mathbf{b}_\beta \quad (109a)$$

$$\text{B.C.} \quad -\mathbf{n}_{\beta\sigma} \cdot (D_\beta \nabla \mathbf{b}_{S\beta} + D_{T\beta} \nabla \mathbf{b}_\beta) = \mathbf{n}_{\beta\sigma} \cdot D_{T\beta} \quad \text{at } A_{\beta\sigma} \quad (109b)$$

$$\mathbf{b}_{S\beta}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_{S\beta}(\mathbf{r}), \quad i = 1, 2, 3 \quad \text{and} \quad \langle \mathbf{b}_{S\beta} \rangle^\beta = 0 \quad (109c)$$

and the resulting macro-scale dispersion equation is

$$\frac{\partial \varepsilon_\beta \langle c_\beta \rangle^\beta}{\partial t} + \nabla \cdot (\varepsilon_\beta \langle \mathbf{v}_\beta \rangle^\beta \langle c_\beta \rangle^\beta) = \nabla \cdot (\varepsilon_\beta \mathbf{D}_{T\beta}^* \cdot \nabla \langle c_\beta \rangle^\beta + \varepsilon_\beta \mathbf{D}_{T\beta}^* \cdot \nabla \langle T \rangle) \quad (110)$$

where the effective thermal dispersion tensor is given by

$$\mathbf{D}_{T\beta}^* = D_\beta \left(\frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{S\beta} dA \right) + D_{T\beta} \left(\mathbf{I} + \frac{1}{V_\beta} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{T\beta} dA \right) - \langle \tilde{\mathbf{v}}_\beta \mathbf{b}_{S\beta} \rangle^\beta \quad (111)$$

Many interesting features may be obtained from this analysis: (i) in the diffusive regime one obtains the important result that $\frac{D_{\beta}^*}{D_{\beta}} = \frac{D_{T\beta}^*}{D_{T\beta}}$ ([139, 147]), (ii) effect of pore-scale convection is complex and may lead to macro-scale thermodiffusion effects of sign opposite to the molecular value as shown in [139].

5.3.2 Strong couplings

In many cases, however, there is a *strong coupling* and it is difficult to find a complete closure. This, of course, leaves the door open for the use of heuristic or semi-heuristic models, which is in fact the status of many models used in porous media physics. To illustrate this problem, let us consider transport in porous media with intense phase change. A typical application would be boiling occurring when cooling the hot debris bed of a nuclear reactor after a loss-of-coolant accident (Loca). So far, closures have been proposed in which the momentum transport is treated independently. Practical models make use of generalized Darcy's laws, or Forchheimer extensions ([148–150]). These models remain largely heuristic and are not entirely supported by the classical two-phase upscaling developments ([79, 80, 91, 93]), which do not take into account the specifics of the phase repartition when boiling occurs in the porous medium. The need for non-equilibrium heat transfer model for Loca modeling has been recognized long ago ([151, 152]). The macro-scale model has usually the form of a three-temperature model. A limited closure can be found for such a model assuming a quasi-static gas-liquid interface ([132]). In this context, calculations of the effective properties suggested a significant difference between the values for a wet solid surface, so-called *slg* configuration, which would occur when boiling is not important, compared to a *sgl* configuration with a vapour film near the solid surface. Moreover, pore-scale nucleate boiling does not certainly fit with a quasi-static interface assumption! Therefore, it is expected that both two-phase and energy models should be impacted by the phase change process taking place within the pores. Experimental evidence interpreted through a three-temperature model ([153]) suggests that there is indeed an impact of the two-phase configuration on the effective properties and that, at least for the heat exchange coefficients, Nukiyama curves ([154]) specific to porous media configurations should be introduced [155]. It is important to understand at this point that intense boiling implies rapidly varying phase configuration with time. Therefore, the use of specific porous media Nukiyama's curves means precisely that the macro-scale equations are in fact spatially and time averaged.

The question of upscaling transport equations with a spatial and time averaging is still an open problem. It has mainly received some attention in the case of turbulent flows in porous media, while it is certainly of utmost importance in the case of multi-phase flow, not only for boiling as emphasized above but also for non quasi-static flows. Mathematically speaking the spatial and time averaging operators commute as is discussed in [156]. However, if one attempts to develop a closure, it seems that a sequential approach is the most practical, as discussed in Sec. 3.2 for the case of the one-phase momentum equation. Since closure involves approximations, the resulting schemes do not necessarily commute. Which sequential averaging is the best? This is a difficult question that has received various answers in the literature. The coupling of turbulence effects with mass and heat transport is clearly an open problem which is the focus of current work [75].

6.0 CONCLUSIONS

The problem of heat and mass transfer in porous media leads to several different classes of problems with more or less coupling between the mass, momentum and energy balance equations. Hence, the association of this diversity with the multi-scale aspect leads to various types of models, one to N-equations models of various mathematical forms, mixed or hybrid models. This multi-scale aspect has been the focus of this lecture and these questions have been reviewed for classical transport problems.

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