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Michel Quintard

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Transfers in Porous Media

M. Quintard

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Université de Toulouse; INPT, UPS; IMFT (Institut de Mécanique des Fluides de Toulouse); Allée Camille Soula, F-31400 Toulouse, France

and CNRS; IMFT; F-31400 Toulouse, France

Abstract

Modeling heat transfer 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 as it is outlined in a brief review based on a simple heat conduction example proposed in the first part of this paper. The more general and classical problem of heat transfer in porous media is reviewed in this paper with the emphasis on the fact that different behaviors and hence different models emerge at a given macro-scale, depending on the interplay of the various characteristic times and lengths characterizing the problem. Various classes of models are discussed and their relationships outlined. Extensions to more complicated problems of heat transfer in porous media are discussed: coupling with mass diffusion, effect of heat sources, radiation, boiling, etc.

Keywords: Porous media, Multiphase, Upscaling methods

1 Introduction

Heat transfer in porous media is central in many applications involving industrial devices (chemical engineering, heat exchangers, nuclear reactor, etc.) as well as complex geological formations (in situ combustion and pyrolysis, geothermal sites, etc.). As a consequence, such heat transfer problems are often characterized by highly non-linear couplings with many different scales involved. The most common multi-scale feature is illustrated in Fig. 1, which represent a typical porous medium two-scale description. The lower-scale is the pore-scale where phases are differentiated, 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 scale is related to the classical discussion about the existence of a Representative Elementary Volume (Hill (1963), Bear (1972))). In the sequel of this presentation, on will assume that all scales involved are nicely separated, 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, such as network modeling (Dullien (1979)), must be used. Another class of porous media which will not be considered in this paper calls also for specific approaches: those with a fractal structure over a large range of scales (Sahimi (1996)).

In the above paragraph, the need for macro-scale models when dealing with practical applications has been emphasized. Of course, one may introduce ad hoc or heuristic models, and, as a matter of fact, this is the case for many of the classical macro-scale models used in the engineering practice. However, it is often more reliable to have at its disposal a comprehensive framework that links the known pore-scale physics to the associated macro-scale theory. Not only this provides a strong basis for developing correct (physically speaking) models,

but it also offers a guidance for developing new, original models for surging problems. Because of the problem complexity, mainly due to the multi-scale aspects outlined above, there is not a single route from one pore-scale problem to a macro-scale model. Indeed, two major issues must be addressed:

- Given the interplay between the different mechanisms and the potential contrast of transport properties (such as diffusivities for instance), several behaviors may be observed requiring specific macro-scale models. This is the case with the discussion in Sec. 3 about non-equilibrium and equilibrium models,
- Similarly, it is not surprising to find that many different methods have been designed to deal with the upscaling aspects.

This paper offers a review of these two problems. The first section proposes a brief overview of the different available upscaling techniques. Next, the potential for different macro-scale models will be illustrated for the classical porous medium heat transfer problem. Finally, indications will be given on open or modern problems which are the subject of current research in the area of heat transfer in porous media. Of course, the format of this paper does not allow for writing an encyclopedia, nor a thorough comprehensive review. It is modestly expected that keys will be provided for understanding what is at stake when working on such upscaling problems.

2 Upscaling methodologies: a brief overview

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

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

where T is the temperature.

This equation is also equivalent, mathematically speaking, 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 sections are in fact connected to these latter problems and not heat transfer. This meaningless difference will not be stressed in the context of this review.

2.1 Obtaining a macro-scale theory through volume averaging

How to define macro-scale variables and how to obtain macro-scale equations? Macro-scale variables are in some broad sense 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 (Marle (1965), Whitaker (1967), Slattery (1967), Marle (1982)). In this framework, one would define the macro-scale temperature field by

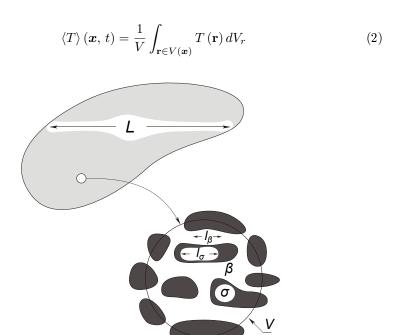


Figure 1: Multiple-scale description of a porous medium.

where V(x) is a volume centered at x and of volume V. 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 Marle (1965), Mls (1987), Marle (1982) and the series of paper Quintard and Whitaker (1994e,d,c,b,a) for a better understanding of the problem. A macro-scale equation could be obtained from averaging of the pore-scale equation, and this would lead to

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

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. A work-flow has been proposed to solve this problem and that makes use of the following steps:

Step 1: define temperature deviation

$$T = \langle T \rangle + \tilde{T} \tag{4}$$

Step 2: develop averaged equation

$$\nabla \cdot \left\langle \mathbf{k} \left(\boldsymbol{x} \right) \cdot \left(\nabla \left\langle T \right\rangle + \nabla \tilde{T} \right) \right\rangle = 0 \tag{5}$$

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

$$\nabla \cdot \left(\mathbf{k} \left(\boldsymbol{x} \right) \cdot \nabla \tilde{T} \right) = -\nabla \cdot \left(\mathbf{k} \left(\boldsymbol{x} \right) \cdot \nabla \left\langle T \right\rangle \right) \tag{6}$$

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

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

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

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

completed by (not discussed in this paper)

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

where the last equation corresponds to periodicity conditions.

Step 5: Obtain a closed form of the macro-scale equation, i.e.,

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

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

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

The upscaling process provides not only the form of the equation compatible with the assumptions made, but also a way of calculating the effective property through the knowledge of pore-scale characteristics. While in the past such calculations were considered as too cumbersome 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 (Adler (1994)). Indeed, several commercial softwares for CT-scan treatment offer tools to compute the most simple effective properties (diffusivity, permeability, ...).

The above work-flow is a schematic presentation for a simple problem. The reader may find a more comprehensive presentation in Whitaker (1999). Other techniques were devised to interpret the additional terms that appear when balance equations are averaged. For instance, this can be achieved heuristically (Slattery (1967), Bear and Bachmat (1990)) 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 Hsu (1999), Nakayama et al. (2001)), which offers, through a less complex closure, a possible way of dealing with complicated coupled problems.

2.2 Other point of views

Different routes have been proposed to achieve the same goal, which differ by many different aspects. In particular, one should look at the definition of the macro-scale variable. The reader will find below a brief overview of the major branches.

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, with the macroscale fields 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 beyond the scope of this paper to provide a complete picture, and we will, for simplicity, outline the development using asymptotic developments for periodic domains, as in Sanchez-Palencia (1970, 1971), Ene and Sanchez-Palencia (1975), Babuška (1976), Bensoussan et al. (1978), Ene and Sanchez-Palencia (1981), Auriault (1983), Mikelic and Primicerio (1994), Auriault (1983) and many other contributions. One may refer to Tartar (2009) for the presentation of a different, less restrictive view. Basically, the temperature field will be looked at in terms of a multi-scale expansion involving ${\bf x}$ and ${\bf y}$ treated as independent variables in the limit $\epsilon \to 0$ such as

$$T(\mathbf{x}) = \sum_{i} T_{i} \left(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon} \right) \epsilon^{i}$$
(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 we assume that $\mathbf{k}(\mathbf{x}, \mathbf{y}) = \mathbf{k}(\mathbf{y})$).

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

$$\nabla_{y} \cdot (\mathbf{k} \cdot \nabla_{y} T_{1}) + \nabla_{y} \cdot (\mathbf{k} \cdot \nabla_{x} T_{0}) = 0$$
(13)

which suggests a solution of the form

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

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

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

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

$$\nabla_x \cdot (\mathbf{K}_{eff} \cdot \nabla_x T_0) = 0 \tag{16}$$

where the effective thermal conductivity is given by

$$\mathbf{K}_{eff} = \langle \mathbf{k} \cdot (\mathbf{I} + \nabla_y \mathbf{b}) \rangle \tag{17}$$

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 Bourgeat et al. (1988) and a more thorough analysis by Davit et al. (2013), Davit and Quintard (2015). One sees from the two developments that:

- the operational definition of the macro-scale variables is different, while one may recognize that $\langle T \rangle = \left\langle \sum_i T_i \left(\mathbf{x}, \mathbf{y} = \frac{\mathbf{x}}{\epsilon} \right) \epsilon^i \right\rangle = T_0$,
- 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} ,

• 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 (Matheron (1965), Gelhar (1986), Dagan (1989), Dagan and Neuman (1997)). 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.

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

While there is not a direct connection between $T^e = E(T)$ and $\langle T \rangle$, the link between the stochastic point of view and spatial averaging comes from an ergodicity assumption which is most often (but not always, Dagan (1990)!) considered when building the ensemble statistical properties. 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 of for the homogenization theory. However, some methods make use of a perturbation analysis in terms of the covariance of k (see Beran (1968), Dagan (1989)), which is reminiscent of the way a "closure" is obtained with the previously introduced two-scale methods. One may refer to Wood et al. (2003)

for a comparison between the stochastic analysis of the problem of dispersion in Fiori and Dagan (2000) and results obtained with the use of a volume averaging theory from Quintard et al. (2001).

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 (Dagan (1989)).

While this also can be done through the examination of 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 Dagan (1989), chap. 2) by looking at the expectation for the flow energy that

$$K_H \le K_{eff} \le K_A \tag{19}$$

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. Wiener's bounds (Wiener (1912)), 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 Hashin and Shtrikman (1963) or a more thorough discussion in Torquato (2002).

Variants

The method of volume averaging has triggered many variants. For example, Marle (1965, 1967) proposed to justify Darcy's law using irreversible thermodynamics. The idea that macroscale models should be compatible with the principles of thermodynamics was not new (Mokadam (1961), Scheidegger (1961), Biot (1962)), but the coupling with volume averaging produced a specific methodology used by several authors (for instance Hassanizadeh and Gray (1979), Ben-

nethum and Cushman (1996), ...). Such a methodology is also reminiscent of the theory of mixtures (see Bowen (1976)). 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.

The method of moments for spatially periodic media, as developed in Brenner (1980), Kitanidis (1992), 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 paper 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 presented for more complex heat transfer in porous media problems. Given the format allowed for this contribution, we will not detail the steps for the upscaling developments but rather put the emphasis 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 The classical heat transfer in porous media problem

In this section, major results are reviewed 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. 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. The one phase flow upscaling problem leads to the classical Darcy's law (see Ene and Sanchez-Palencia (1975), Whitaker (1986a)) when the pore-scale Reynolds number is small enough. Inertia terms play a role when the pore-scale Reynolds number increases and a generalized Forchheimer equation may be used (Wodié and Lévy (1991), Skjetne and Auriault (1999), Whitaker (1996)). It has also been shown in Lasseux et al. (2011) that this Forchheimer model is relatively robust and accurate. 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

$$(\rho c_p)_{\beta} \frac{\partial T_{\beta}}{\partial t} + (\rho c_p)_{\beta} \mathbf{v}_{\beta} \cdot \nabla T_{\beta} = \nabla \cdot (k_{\beta} \nabla T_{\beta}) \quad \text{in } V_{\beta}$$
 (20)

$$T_{\beta} = T_{\sigma}$$
 at $A_{\beta\sigma}$ (21)

$$\mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla T_{\beta} = \mathbf{n}_{\beta\sigma} \cdot k_{\sigma} \nabla T_{\sigma} \quad \text{at } A_{\beta\sigma}$$
 (22)

$$(\rho c_p)_{\sigma} \frac{\partial T_{\sigma}}{\partial t} = \nabla \cdot (k_{\sigma} \nabla T_{\sigma}) \quad \text{in } V_{\sigma}$$
 (23)

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.

The objective of this section 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 (Whitaker (1999)) as a mere guideline. Additional literature will be cited to complete the learning process for those interested in the upscaling details.

3.1 The structure of the micro-macro coupled problem

As schematically described in Sec. 2.1, one needs to develop the coupled macroscale and micro-scale equations. It is only listed below the averaged and deviation equation for the β -phase as well as the boundary conditions at $A_{\beta\sigma}$. The mathematical development makes extensive use of the classical averaging theorems (see Marle (1982) for a proof using the theory of distribution) given by

$$\langle \nabla \psi_{\beta} \rangle = \nabla \langle \psi_{\beta} \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_{\beta} dA$$
 (24a)

$$\langle \nabla \cdot \mathbf{A}_{\beta} \rangle = \nabla \cdot \langle \mathbf{A}_{\beta} \rangle + \frac{1}{V} \int_{A_{\beta\sigma}}^{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_{\beta} dA$$
 (24b)

$$\left\langle \frac{\partial \psi_{\beta}}{\partial t} \right\rangle = \frac{\partial \left\langle \psi_{\beta} \right\rangle}{\partial t} - \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{w}_{\beta\sigma} \psi_{\beta} dA \tag{24c}$$

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

Averaging of Eq. 20 leads to

$$\underbrace{\varepsilon_{\beta}(\rho c_{p})_{\beta} \frac{\partial \langle T_{\beta} \rangle^{\beta}}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_{\beta}(\rho c_{p})_{\beta} \langle \mathbf{v}_{\beta} \rangle^{\beta} \cdot \nabla \langle T_{\beta} \rangle^{\beta}}_{\text{convection}} = \underbrace{\nabla \cdot \left[k_{\beta} \left(\varepsilon_{\beta} \nabla \langle T_{\beta} \rangle^{\beta} + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_{\beta} \, dA \right) \right]}_{\text{conduction/tortuosity}} - \underbrace{\left(\rho c_{p} \right)_{\beta} \nabla \cdot \langle \tilde{\mathbf{v}}_{\beta} \tilde{T}_{\beta} \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_{\beta} \nabla T_{\beta} \, dA}_{\text{interfacial flux}} \right] \tag{25}$$

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 notations have been adopted

$$\varepsilon_{\beta} = \frac{V_{\beta}}{V} = 1 - \varepsilon_{\sigma} \; ; \; \langle T_{\beta} \rangle = \varepsilon_{\beta} \langle T_{\beta} \rangle^{\beta}$$
 (26)

$$T_{\alpha} = \langle T_{\alpha} \rangle^{\alpha} + \tilde{T}_{\alpha} \tag{27}$$

for the β -phase volume fraction, ε_{β} , the intrinsic averaged temperature, $\langle T_{\beta} \rangle^{\beta}$, and the temperature deviation \tilde{T}_{α} .

The micro-scale equation may be written as

$$(\rho c_p)_{\beta} \frac{\partial \tilde{T}_{\beta}}{\partial t} + (\rho c_p)_{\beta} \tilde{\mathbf{v}}_{\beta}.\nabla \langle T_{\beta} \rangle^{\beta} + (\rho c_p)_{\beta} \mathbf{v}_{\beta}.\nabla \tilde{T}_{\beta} = \nabla.(k_{\beta} \nabla \tilde{T}_{\beta})$$

$$-\varepsilon_{\beta}^{-1} \nabla. \left(k_{\beta} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_{\beta} dA \right) - \varepsilon_{\beta}^{-1} k_{\beta} \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma}.\nabla \tilde{T}_{\beta} dA$$
(28)

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

$$\tilde{T}_{\beta} = \tilde{T}_{\sigma} - \underbrace{\left(\left\langle T_{\beta}\right\rangle^{\beta} - \left\langle T_{\sigma}\right\rangle^{\sigma}\right)}_{\text{source term}}$$
(29)

$$-\mathbf{n}_{\beta\sigma}.k_{\beta}\nabla \tilde{T}_{\beta} - \underbrace{\mathbf{n}_{\beta\sigma}.k_{\beta}\nabla \langle T_{\beta}\rangle^{\beta}}_{\text{source term}} = -\mathbf{n}_{\beta\sigma}.k_{\sigma}\nabla \tilde{T}_{\sigma} - \underbrace{\mathbf{n}_{\beta\sigma}.k_{\sigma}\nabla \langle T_{\sigma}\rangle^{\sigma}}_{\text{source term}}$$
(30)

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

3.2 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, one will 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.

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, i.e.,

$$\left(\frac{(\rho c_p)_{\beta} l_{\beta}^2}{k_{\beta}} \approx \frac{(\rho c_p)_{\sigma} l_{\sigma}^2}{k_{\sigma}}\right) \ll \left(\frac{\varepsilon_{\beta} (\rho c_p)_{\beta} L^2}{K_{\beta}^*} \approx \frac{\varepsilon_{\sigma} (\rho c_p)_{\sigma} L^2}{K_{\sigma}^*}\right)$$
(31)

As a consequence, the two macro-scale temperatures are close enough so one can introduce the following approximation, characteristic of the so-called localequilibrium case,

$$\langle T_{\beta} \rangle^{\beta} = \langle T_{\sigma} \rangle^{\sigma} = \langle T \rangle \tag{32}$$

with the total heat for the mixture given by

$$\varepsilon_{\beta} \left(\rho c_{p} \right)_{\beta} \left\langle T_{\beta} \right\rangle^{\beta} + \varepsilon_{\sigma} \left(\rho c_{p} \right)_{\sigma} \left\langle T_{\sigma} \right\rangle^{\sigma} = \left(\rho c_{p} \right)^{*} \left\langle T \right\rangle \tag{33}$$

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 (Carbonell and Whitaker (1984))

$$\tilde{T}_{\beta} = \mathbf{b}_{\beta}(\mathbf{y}).\nabla \langle T \rangle (\mathbf{x}, t) + \dots$$
 (34a)

$$\tilde{T}_{\sigma} = \mathbf{b}_{\sigma}(\mathbf{y}).\nabla \langle T \rangle (\mathbf{x}, t) + \dots$$
 (34b)

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

$$(\rho c_p)_{\beta} \tilde{\mathbf{v}}_{\beta} + (\rho c_p)_{\beta} \mathbf{v}_{\beta}.\nabla \mathbf{b}_{\beta} = k_{\beta} \nabla^2 \mathbf{b}_{\beta} \text{ in } V_{\beta}$$
(35a)

B.C.1
$$-\mathbf{n}_{\beta\sigma}.k_{\beta}\nabla\mathbf{b}_{\beta} - \mathbf{n}_{\beta\sigma}k_{\beta} = -\mathbf{n}_{\beta\sigma}.k_{\sigma}\nabla\mathbf{b}_{\sigma} - \mathbf{n}_{\beta\sigma}k_{\sigma} \text{ at } A_{\beta\sigma}$$
 (35b)

B.C.2
$$\mathbf{b}_{\beta} = \mathbf{b}_{\sigma} \text{ at } A_{\beta\sigma}$$
 (35c)

$$0 = k_{\sigma} \nabla^2 \mathbf{b}_{\sigma} \text{ in } V_{\sigma} \tag{35d}$$

$$\mathbf{b}_{\beta}(\mathbf{x} + \mathbf{l}_{i}) = \mathbf{b}_{\beta}(\mathbf{x}) \; ; \; \mathbf{b}_{\sigma}(\mathbf{x} + \mathbf{l}_{i}) = \mathbf{b}_{\sigma}(\mathbf{x}) \quad i = 1, 2, 3$$
 (35e)

$$\langle \mathbf{b}_{\beta} + \mathbf{b}_{\sigma} \rangle = 0 \tag{35f}$$

Adding Eq. 28 with its σ -phase counterpart, and substituting the deviations by their expressions Eqs. 34, one obtains the following local-equilibrium macroscale equation

$$(\rho c_p)^* \frac{\partial \langle T \rangle}{\partial t} + \varepsilon_\beta (\rho c_p)_\beta \mathbf{U}_\beta \cdot \nabla \langle T \rangle = \nabla \cdot (\mathbf{K}_{eq}^* \cdot \nabla \langle T \rangle)$$
(36)

where the effective thermal conductivity tensor is given by

$$\mathbf{K}_{eq}^{*} = (\varepsilon_{\beta}k_{\beta} + \varepsilon_{\sigma}k_{\sigma})\mathbf{I} + \frac{k_{\beta} - k_{\sigma}}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{\beta} dA - (\rho c_{p})_{\beta} \langle \tilde{\mathbf{v}}_{\beta} \mathbf{b}_{\beta} \rangle^{\beta}$$
(37)

and where $\mathbf{U}_{\beta} = \langle \mathbf{v}_{\beta} \rangle^{\beta}$. The effective thermal conductivity can be estimated experimentally or calculated by solving Eqs. 35 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 Kaviany (1995), Kandula (2011). 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 (Zehner and Schlünder (1970), Shonnard and Whitaker (1989), Oliveira and Kaviany (1999)).

Non-equilibrium models

Non-equilibrium models arise when the contrast between the transport properties of the various phases are not well separated. 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. 3.1 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 involves a time convolution as has been discussed in Moyne (1997) for a pure conductive problem and in Davit et al. (2012) from a more general perspective. The deviations in this framework are expressed as

$$\tilde{T}_{\beta} = \mathbf{b}_{\beta\beta} \star \frac{\partial}{\partial t} \nabla \langle T_{\beta} \rangle^{\beta} + \mathbf{b}_{\beta\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_{\sigma} \rangle^{\sigma} - s_{\beta} \star \frac{\partial}{\partial t} \left(\langle T_{\beta} \rangle^{\beta} - \langle T_{\sigma} \rangle^{\sigma} \right) + \dots$$
(38a)

$$\tilde{T}_{\sigma} = \mathbf{b}_{\sigma\beta} \star \frac{\partial}{\partial t} \nabla \langle T_{\beta} \rangle^{\beta} + \mathbf{b}_{\sigma\sigma} \star \frac{\partial}{\partial t} \nabla \langle T_{\sigma} \rangle^{\sigma} + s_{\sigma} \star \frac{\partial}{\partial t} \left(\langle T_{\sigma} \rangle^{\sigma} - \langle T_{\beta} \rangle^{\beta} \right) + \dots$$
(38b)

where the mapping variables closure problems are time-dependent. The mapping variables relax more rapidly with time than the macro-scale temperatures and one may seek a steady-state closure under the following form (Carbonell and Whitaker (1984), Zanotti and Carbonell (1984), Levec and Carbonell (1985), Quintard and Whitaker (1993), Quintard et al. (1997))

$$\tilde{T}_{\beta} = \mathbf{b}_{\beta\beta}.\nabla \langle T_{\beta} \rangle^{\beta} + \mathbf{b}_{\beta\sigma}.\nabla \langle T_{\sigma} \rangle^{\sigma} - s_{\beta} \left(\langle T_{\beta} \rangle^{\beta} - \langle T_{\sigma} \rangle^{\sigma} \right) + \dots$$
 (39a)

$$\tilde{T}_{\sigma} = \mathbf{b}_{\sigma\beta}.\nabla \langle T_{\beta} \rangle^{\beta} + \mathbf{b}_{\sigma\sigma}.\nabla \langle T_{\sigma} \rangle^{\sigma} + s_{\sigma} \left(\langle T_{\sigma} \rangle^{\sigma} - \langle T_{\beta} \rangle^{\beta} \right) + \dots$$
 (39b)

where the mapping variables are the limit of the time dependent closure for $t \to 0$. As an example, the problem for the mapping variables s_{β} and s_{σ} is given by

$$(\rho c_p)_{\beta} \mathbf{v}_{\beta}. \nabla s_{\beta} = k_{\beta} \nabla^2 s_{\beta} - \varepsilon_{\beta}^{-1} h_{\beta} \quad , \text{ in } V_{\beta}$$
 (40a)

B.C.1.
$$\mathbf{n}_{\beta\sigma}.k_{\beta}\nabla s_{\beta} = \mathbf{n}_{\beta\sigma}.k_{\sigma}\nabla s_{\sigma}$$
 , at $A_{\beta\sigma}$ (40b)

B.C.2.
$$s_{\beta} = 1 + s_{\sigma}$$
, at $A_{\beta\sigma}$ (40c)

$$0 = k_{\sigma} \nabla^2 s_{\sigma} + \varepsilon_{\sigma}^{-1} h_{\sigma} \quad , \text{ in } V_{\sigma}$$
 (40d)

$$s_{\beta}(\mathbf{r} + \mathbf{l}_i) = s_{\beta}(\mathbf{r}), \quad s_{\sigma}(\mathbf{r} + \mathbf{l}_i) = s_{\sigma}(\mathbf{r}) \quad , \quad i = 1, 2, 3$$
 (40e)

$$\langle s_{\beta} \rangle = 0 \quad ; \quad \langle s_{\sigma} \rangle = 0$$
 (40f)

$$h_{\beta} = \langle \mathbf{n}_{\beta\sigma}.k_{\beta}\nabla s_{\beta} \delta_{\beta\sigma} \rangle \quad ; \quad h_{\sigma} = -\langle \mathbf{n}_{\sigma\beta}.k_{\sigma}\nabla s_{\sigma} \delta_{\beta\sigma} \rangle = h_{\beta} = h_{2eq}$$
 (40g)

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 integrodifferential 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

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

$$(41a)$$

$$\varepsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma} \frac{\partial \left\langle T_{\sigma}\right\rangle^{\sigma}}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \left\langle T_{\beta}\right\rangle^{\beta} - \mathbf{u}_{\sigma\sigma} \cdot \nabla \left\langle T_{\sigma}\right\rangle^{\sigma} =$$

$$\nabla \cdot \left(\mathbf{K}_{\sigma\beta}^{*} \cdot \nabla \left\langle T_{\beta}\right\rangle^{\beta} + \mathbf{K}_{\sigma\sigma}^{*} \cdot \nabla \left\langle T_{\sigma}\right\rangle^{\sigma}\right) - h_{2eq} \left(\left\langle T_{\sigma}\right\rangle^{\sigma} - \left\langle T_{\beta}\right\rangle^{\beta}\right) \tag{41b}$$

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

$$\mathbf{K}_{eq}^* = \mathbf{K}_{\beta\beta}^* + \mathbf{K}_{\beta\sigma}^* + \mathbf{K}_{\sigma\beta}^* + \mathbf{K}_{\sigma\sigma}^*$$
 (42)

Simpler closures may be used depending on the assumptions made on the physical characteristics of the problem (Hsu (1999), DeGroot and Straatman (2011)). If one drops the additional convective and cross-terms¹, one recovers the traditional two-equation model often used in the literature (Schlünder (1975), Glatzmaier and Ramirez (1988)). The heat exchange coefficient, h_{2eq} , provides one single relaxation time as opposed to the full spectrum discussed in the introduction to this section. Hence, this is not really an intrinsic property of the porous medium and its value depends on the theory used to define it or the measurement method. Indeed, several values have been proposed in the literature and the reader is referred to Landereau et al. (2001) for a more thorough discussion 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 Eqs. 40 plays a fundamental role, as will be shown in Sec. 3.2, and is related to the harmonic mean of the eigenvalues.

Another problem comes from the periodicity conditions which are often used when solving closure problems (as is the case in Eq. 40e). If one takes, as an analogy of a porous medium problem, heat transfer in a tube (the Graetz problem), such conditions are compatible with the established regime (Golfier et al. (2002)). 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. Taking into account these entrance effects would lead to a non-local (in space) analysis, i.e., the transport equation and especially the effective properties depend also on the flow and boundary conditions far from the local position. It also contributes to the differences encountered in the literature between the different correlations or estimates of the heat exchange coefficient.

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 Golfier et al. (2002)

The heat exchange coefficient is also often written as

$$h_{2eq} = a_v h (43)$$

where a_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, if one assumes that such a boundary condition exists at the pore-scale, one recovers from the upscaling process a two-equation model with an exchange terms written like Eq. 43 (Pernin (1984), Auriault and Lewandowska (1997)). 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. 40a through 40g, involves a diffusive process which will generate cut-off or smoothing effects for rough or fractal surfaces. Therefore, Eq. 43 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 (Whitaker (1991), Quintard and Whitaker (1993), Amiri and Vafai (1994), Quintard and Whitaker (1995), Minkowycz et al. (1999), Vadasz (2005)). 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 a little bit more complex and depends on the geometry and topology of the unit cell (Quintard and Whitaker (1993)), the boundary value problem solved (Vafai and Sozen (1990), Vadasz (2005)), the processes involved, for instance natural convection (Rees and Pop (2005)), phase change (Soezen and Vafai (1990), Duval et al. (2004)), the coupling with reactive transport (Fatehi and Kaviany (1997), Oliveira and Kaviany (2001)), etc...

Asymptotic behavior and One-Equation Non-Equilibrium model

It has been shown in Zanotti and Carbonell (1984), Levec and Carbonell (1985), Davit et al. (2012) that the two equation model can be approximated asymptotically as $t \to \infty$ for a uniform 1D flow by a classical heat equation

$$\left(\varepsilon_{\beta}\left(\rho c_{p}\right)_{\beta}+\varepsilon_{\sigma}\left(\rho c_{p}\right)_{\sigma}\right)\frac{\partial\left\langle T\right\rangle^{\beta\sigma}}{\partial t}+\varepsilon_{\beta}\left(\rho c_{p}\right)_{\beta}\left\langle \mathbf{v}_{\beta}\right\rangle^{\beta}\cdot\nabla\left\langle T\right\rangle^{\beta\sigma}=\nabla\cdot\left(\mathbf{K}_{\infty}^{*}\cdot\nabla\left\langle T\right\rangle^{\beta\sigma}\right)$$
(44)

where

$$\langle T \rangle^{\beta \sigma} = \frac{\left(\epsilon_{\beta} \left(\rho c_{p}\right)_{\beta} \langle T_{\beta} \rangle^{\beta} + \epsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma} \langle T_{\sigma} \rangle^{\sigma}\right)}{\left(\epsilon_{\beta} \left(\rho c_{p}\right)_{\beta} + \epsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma}\right)}$$
(45)

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

$$\mathbf{K}_{\infty}^{*} = \mathbf{K}_{eq}^{*} + \frac{1}{h_{2eq}} \frac{\left(\varepsilon_{\beta} \left(\rho c_{p}\right)_{\beta} \varepsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma}\right)^{2}}{\left(\varepsilon_{\beta} \left(\rho c_{p}\right)_{\beta} + \varepsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma}\right)^{2}} \mathbf{U}_{\beta} \mathbf{U}_{\beta}$$
(46)

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, as discussed in Levec and Carbonell (1985), Davit et al. (2012). This merely means that the front spreading tends to mask the lag between the two average temperatures. Another important discovery is that a direct closure can be found based on $\langle T \rangle^{\beta\sigma}$ (Moyne et al. (2000), Quintard et al. (2001), Davit et al. (2010)) if one looks at the pore-scale temperature fields through the following decomposition

$$\hat{T}_{\beta} = T_{\beta} - \langle T \rangle^{\beta \sigma} \approx \mathbf{b}_{\beta}^{\infty} . \nabla \langle T \rangle^{\beta \sigma} ; \hat{T}_{\sigma} = T_{\sigma} - \langle T \rangle^{\beta \sigma} \approx \mathbf{b}_{\sigma}^{\infty} . \nabla \langle T \rangle^{\beta \sigma}$$
 (47)

It was proven numerically and analytically (Quintard et al. (2001), Davit et al. (2010)) that the resulting non-equilibrium one-equation model is similar to Eq. 44 and that the two effective thermal dispersion tensors (two-equation asymp-

totic behaviour and one-equation non-equilibrium closure) are equal if the heat exchange coefficient is the one from the closure provided by Eqs. (40). To be clear enough, the use of other estimates (see Landereau et al. (2001)) 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 Wang and Wei (2008) 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 (Sabatier et al. (2007)).

Discussion

At this point, one already has at hand several models for the *same* initial pore-scale problem! The reader is referred to Davit et al. (2010) (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 Davarzani et al. (2010) (this problem is also revisited in Davit and Quintard (2015)). Fig. 2 reproduces 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 the solution calls for a local non-equilibrium treatment,
- the asymptotic behavior is later observed, 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, one observes that the conditions revert to local equilibrium! Hence 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, it is important to understand that one has to be careful when recommending the exclusive use of such and such model, as is sometimes the case in the literature. The proposed 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 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 have been already emphasized, i.e., it has only a single characteristic time for describing the fluid-solid temperature relaxation! This drawback may in principle be overcome through the use of the full model with convolution products. However, convolution products are not handy for numerical

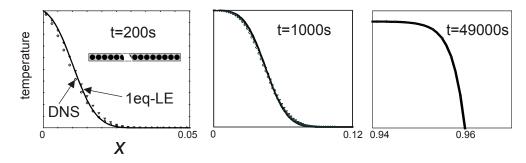


Figure 2: Transient evolution of macro-scale models (adapted from Davarzani et al. (2010))

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 Haggerty and Gorelick (1995) 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 convolution products.

A final class of model, called mixed or hydrid 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. (30) may be approximated by

$$\langle T_{\beta} \rangle^{\beta} + \underbrace{\tilde{T}_{\beta}}_{O(\frac{l_{\beta}}{L}\langle T_{\beta} \rangle^{\beta})} = T_{\sigma} \qquad \Rightarrow \qquad \underbrace{\langle T_{\beta} \rangle^{\beta}}_{macro-scale} = \underbrace{T_{\sigma}}_{micro-scale}$$
 (48)

The final model combines a micro-scale diffusion equation coupled through Eq. (48) to a macro-scale equation in which the effective thermal dispersion tensor is the one provided by Eqs. (35) 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 Debenest and Quintard (2008). Another type of mixed model may be introduced when sharp thermal fronts are encountered as in Debenest et al. (2005) 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. 3 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.

4 Extensions and open problems

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

4.1 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 Quintard and Whitaker (2000) 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 models. The effect of the heterogeneous source, Ω , is more tricky and requires an additional closure problem that allows for the distribution of the heat source between the

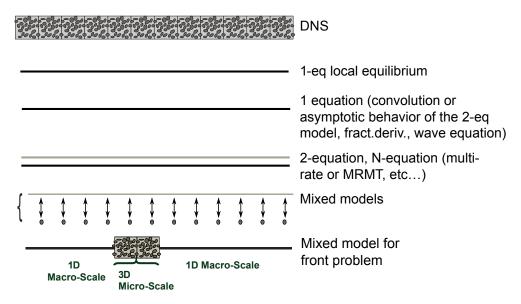


Figure 3: Multiple-scale description of a porous medium.

two equations, i.e., the two-temperature model becomes

$$\varepsilon_{\beta} \left(\rho c_{p}\right)_{\beta} \frac{\partial \left\langle T_{\beta}\right\rangle^{\beta}}{\partial t} + \left(\rho c_{p}\right)_{\beta} \left\langle \mathbf{v}_{\beta}\right\rangle . \nabla \left\langle T_{\beta}\right\rangle^{\beta} - \mathbf{u}_{\beta\beta} . \nabla \left\langle T_{\beta}\right\rangle^{\beta} - \mathbf{u}_{\beta\sigma} . \nabla \left\langle T_{\sigma}\right\rangle^{\sigma} = \\
\nabla . \left(\mathbf{K}_{\beta\beta}^{*} . \nabla \left\langle T_{\beta}\right\rangle^{\beta} + \mathbf{K}_{\beta\sigma}^{*} . \nabla \left\langle T_{\sigma}\right\rangle^{\sigma}\right) - h_{2eq} \left(\left\langle T_{\beta}\right\rangle^{\beta} - \left\langle T_{\sigma}\right\rangle^{\sigma}\right) + a_{v} \xi \Omega \qquad (49a)$$

$$\varepsilon_{\sigma} \left(\rho c_{p}\right)_{\sigma} \frac{\partial \left\langle T_{\sigma}\right\rangle^{\sigma}}{\partial t} - \mathbf{u}_{\sigma\beta} . \nabla \left\langle T_{\beta}\right\rangle^{\beta} - \mathbf{u}_{\sigma\sigma} . \nabla \left\langle T_{\sigma}\right\rangle^{\sigma} = \nabla . \left(\mathbf{K}_{\sigma\beta}^{*} . \nabla \left\langle T_{\beta}\right\rangle^{\beta} + \mathbf{K}_{\sigma\sigma}^{*} . \nabla \left\langle T_{\sigma}\right\rangle^{\sigma}\right)$$

$$-h_{2eq} \left(\left\langle T_{\sigma}\right\rangle^{\sigma} - \left\langle T_{\beta}\right\rangle^{\beta}\right) + a_{v} \left(1 - \xi\right) \Omega + \varepsilon_{\sigma} \Phi_{\sigma} \qquad (49b)$$

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 Quintard and Whitaker (2000), Davit and Quintard (2015) shows that $\xi \to 0$ when $k_{\sigma}/k_{\beta} \to \infty$ which leads to the heuristic equation in which all the produced heat is affected to the solid phase (Oliveira and Kaviany (2001)). 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 (Leroy et al. (2013)).

The coupling with mass transfer and reaction is often treated with some sort of decoupling (Fatchi and Kaviany (1997), Oliveira and Kaviany (2001)). Indeed, if one assumes that the mass reaction rate is of the form

$$r_{\beta} = F\left(c_{\beta}, T_{\beta}\right) = F\left(\langle c_{\beta} \rangle^{\beta}, \langle T_{\beta} \rangle^{\beta}\right) + \frac{\partial F}{\partial c_{\beta}} \left(\langle c_{\beta} \rangle^{\beta}, \langle T_{\beta} \rangle^{\beta}\right) \tilde{c}_{\beta} + \frac{\partial F}{\partial T_{\beta}} \left(\langle c_{\beta} \rangle^{\beta}, \langle T_{\beta} \rangle^{\beta}\right) \tilde{T}_{\beta} + \cdots$$
(50)

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

$$r_{\beta} = F\left(c_{\beta}, T_{\beta}\right) = F\left(\left\langle c_{\beta}\right\rangle^{\beta}, \left\langle T_{\beta}\right\rangle^{\beta}\right)$$
 (51)

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 (Fatehi and Kaviany (1997)) or even call for direct numerical simulations or mixed models (Debenest et al. (2005)). From an upscaling point of view, these problems remain largely open problems.

4.2 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. It has already been emphasized in the above subsection that coupling between the various transport problems may have to be considered.

Often, weak coupling can be treated following the ideas leading to Eq. (51), 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

$$\frac{\partial c_{\beta}}{\partial t} + \nabla \cdot (c_{\beta} \mathbf{v}_{\beta}) = \nabla \cdot (D_{\beta} \nabla c_{\beta} + D_{T\beta} \nabla T_{\beta})$$
 (52)

B.C.1
$$\mathbf{n}_{\beta\sigma}$$
. $(D_{\beta}\nabla c_{\beta} + D_{T\beta}\nabla T_{\beta}) = 0$ at $A_{\beta\sigma}$ (53)

Because of this one-side coupling, the temperature deviations can be estimated from the various closures presented in this paper, i.e., Eqs. (34) or (39). In turn, it can be introduced in the mapping expression for the concentration deviation. For instance, the local equilibrium closure would lead to (Davarzani et al. (2010))

$$\tilde{c}_{\beta} = \mathbf{b}_{C\beta}.\nabla \langle c_{\beta} \rangle^{\beta} + \mathbf{b}_{S\beta}.\nabla \langle T \rangle$$
(54)

The closure problems for $\mathbf{b}_{C\beta}$ is the classical problem leading to the dispersion tensor (Brenner (1980), Carbonell and Whitaker (1983)) while the closure problem for $\mathbf{b}_{S\beta}$ is coupled with the closure problem for \mathbf{b}_{β} described by Eqs. (35). One has

$$\mathbf{v}_{\beta}.\nabla\mathbf{b}_{S\beta} = D_{\beta}\nabla^{2}\mathbf{b}_{S\beta} + D_{T\beta}\nabla^{2}\mathbf{b}_{\beta} \tag{55a}$$

B.C.
$$-\mathbf{n}_{\beta\sigma}.(D_{\beta}\nabla\mathbf{b}_{S\beta} + D_{T\beta}\nabla\mathbf{b}_{\beta}) = \mathbf{n}_{\beta\sigma}.D_{T\beta}$$
 at $A_{\beta\sigma}$ (55b)

$$\mathbf{b}_{S\beta}(\mathbf{r} + \mathbf{l}_i) = \mathbf{b}_{S\beta}(\mathbf{r}) , i = 1, 2, 3 \text{ and } \langle \mathbf{b}_{S\beta} \rangle^{\beta} = 0$$
 (55c)

and the resulting macro-scale dispersion equation is

$$\frac{\partial \varepsilon_{\beta} \langle c_{\beta} \rangle^{\beta}}{\partial t} + \nabla \cdot \left(\varepsilon_{\beta} \langle \mathbf{v}_{\beta} \rangle^{\beta} \langle c_{\beta} \rangle^{\beta} \right) = \nabla \cdot \left(\varepsilon_{\beta} \mathbf{D}_{\beta}^{*} \cdot \nabla \langle c_{\beta} \rangle^{\beta} + \varepsilon_{\beta} \mathbf{D}_{T\beta}^{*} \cdot \nabla \langle T \rangle \right)$$
(56)

where the effective thermal dispersion tensor is given by

$$\mathbf{D}_{T\beta}^{*} = D_{\beta} \left(\frac{1}{V_{\beta}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{S\beta} dA \right) + D_{T\beta} \left(\mathbf{I} + \frac{1}{V_{\beta}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \mathbf{b}_{T\beta} dA \right) - \langle \tilde{\mathbf{v}}_{\beta} \mathbf{b}_{S\beta} \rangle^{\beta}$$
(57)

Many interesting features may be obtained from this analysis: (i) in the diffusive regime one obtains the important result that $\frac{\mathbf{D}_{\beta}^{*}}{D_{\beta}} = \frac{\mathbf{D}_{T\beta}^{*}}{D_{T\beta}}$ (Lacabanne et al. (2002), Davarzani et al. (2010)), (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 Davarzani et al. (2010).

Most of the time, 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 kind of problem, let us consider transport in porous media with intense phase change, like boiling occurring when cooling hot debris bed of 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 (Hardee and Nilson (1977), Catton and Chung (1992), Fichot et al. (2006)). These models remain largely heuristic and are not entirely supported by the classical two-phase upscaling developments (Whitaker (1986b), Auriault (1987), Hassanizadeh and Gray (1993), Panfilov and Panfilova (2005)), 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 (Amarasooriya and Theofanous (1991), Berthoud and Valette (1994)). 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 (Duval et al. (2004)). 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 (Bachrata et al. (2013)) 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 (Nukiyama (1966)) specific to porous media configurations should be introduced. 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 de Lemos (2006). However, if one attempts to develop a closure, it seems that a sequential approach is the most practical. 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. Before discussing this question, let us review the upscaling of the momentum equation when increasing the Reynolds number, Re, which quantifies the importance of inertia effects versus viscous diffusion, and, eventually, the appearance of turbulence. In the limit $Re \rightarrow 0$, upscaling methods give the traditional Darcy's law as already discussed. Increasing Re leads first to a weak inertia regime with a cubic dependence of the pressure loss as shown theoretically in Wodié and Lévy (1991), Mei and Auriault (1991), and many other contributions. This weak inertia regime does not often produce a significant departure from Darcy's law, but it may be observed if accurate measurements are made or when solving numerically Navier-Stokes equations (Firdaouss et al. (1997), Lasseux et al. (2011)). Rapidly, when increasing the Reynolds number, a strong inertia regime occurs, which is often modeled in practice with a Forchheimer equation (Forchheimer (1901)). The classical Forchheimer equation has a quadratic dependence which provides in most cases a satisfactory representation of actual head losses (see discussion in Ergun (1952) for chemical engineering applications, see Lasseux et al. (2011) for a literature review and a discussion of the applicability of the quadratic equation). A generalized Forchheimer equation may be derived through upscaling techniques, as shown in Whitaker (1996) and it has the following form

$$\nabla \cdot \langle \mathbf{v}_{\beta} \rangle = 0 \tag{58}$$

$$\langle \mathbf{v}_{\beta} \rangle = -\frac{1}{\mu_{\beta}} \mathbf{K} \cdot \left(\nabla \langle p_{\beta} \rangle^{\beta} - \rho_{\beta} \mathbf{g} \right) - \mathbf{F} \cdot \langle \mathbf{v}_{\beta} \rangle$$
 (59)

where K is the intrinsic permeability tensor and F the correction tensor. This

latter parameter is obtained through a "closure" problem that involves the local velocity field \mathbf{v}_{β} . Therefore, it is non-linear and depends upon the average velocity in a complex manner, not necessarily linear or cubic (Lasseux et al. (2011)). Indeed, such a generalized Forchheimer equation is useful to describe strong inertia effects (Chauveteau and Thirriot (1967), Skjetne and Auriault (1999)) which may obey power law pressure drops. This model is also useful in the case of unit-cell localized or periodic turbulence, has shown theoretically in Skjetne and Auriault (1999), Soulaine and Quintard (2014). Turbulence is not always of a unit cell periodic type and several attempts have been made to develop macro-scale turbulence models. Two sequential schemes have been discussed in the literature, as illustrated below

I.
$$\mathbf{v}_{\beta} \to \langle \mathbf{v}_{\beta} \rangle \to \overline{\langle \mathbf{v}_{\beta} \rangle}$$
 (60)

II.
$$\mathbf{v}_{\beta} \to \overline{\mathbf{v}_{\beta}} (RANS, ...) \to \langle \overline{\mathbf{v}_{\beta}} \rangle$$
 (61)

Scheme I, favored by Antohe and Lage (1997), Getachew et al. (2000) among others, involves a first spatial averaging. It is assumed that the closed macroscale 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 (Nakayama and Kuwahara (1999), Pedras and de Lemos (2001)). 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 macroscale 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 penetrates several

unit cells into the porous domain and that in this area a porous medium turbulence model is needed (Chandesris et al. (2013)). The coupling of turbulence effects with mass and heat transport is clearly an open problem which is the focus of current research.

5 Conclusions

The problem of heat 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 paper and these questions have been reviewed based on a classical heat transfer problem. It must be emphasized that strong non-linear coupled problems remain largely open questions and deserve further research.

It also must be remembered that several problems of paramount importance have not been addressed in this paper, in particular numerical modeling or the development of appropriate experimental techniques. Developments of new techniques in these area may offer new opportunities to understand and solve more and more of these multi-scale complex problems.

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