



## Heat Transfer in Porous Media: Second-Order Closure and Nonlinear Source Terms

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**Abstract:** Heat transfer in multiscale materials is ubiquitous in natural and engineered systems. These materials are often modeled at a macroscopic scale, where microscopic details are filtered out to reduce numerical and physical complexity. Here, we use the method of volume averaging to upscale heat transfer equations for a saturated porous medium with non-linear bulk and surface sources. This approach leads to the development of a variety of macroscopic models, including a two-temperature model with a second order closure that extends previous results from Quintard and Whitaker [2000]. Effective properties are calculated for model unit-cells (1D, 2D and 3D) and also for a realistic pore-scale geometry obtained using X-ray tomography. The model further features a distribution coefficient that indicates the distribution of the surface heat between the two phases at the macroscale. By comparing computational results for the two-temperature model against direct numerical simulations, we show that this effective distribution coefficient captures well the partitioning of heat, even in the transient regime.

**Mots clés :** porous media, averaging, heat sources

### 1. Introduction

We consider heat transfer in the porous medium schematically represented Figure 1 where a fluid phase,  $\beta$ , flows in a  $\sigma$ -phase solid skeleton. Homogeneous heat sources may be found in both phases, while a heterogeneous heat source may also be considered at the  $\beta\sigma$  interface. Such heat sources may be due to various physical and chemical phenomena: chemical reactions, radioactivity, etc... The pore-scale heat transfer problem which is considered in this paper is written below as

$$(\rho C_p)_\beta \left[ \partial_t T_\beta + \nabla \cdot (\mathbf{v}_\beta T_\beta) \right] = \nabla \cdot (k_\beta \nabla T_\beta) + R_\beta(T_\beta) \text{ in } V_\beta \quad (1)$$

$$\text{BC1} \quad T_\beta - T_\sigma = 0 \text{ at } A_{\beta\sigma}, \quad (2)$$

$$\text{BC2} \quad -\mathbf{n}_{\beta\sigma} \cdot (k_\beta \nabla T_\beta - k_\sigma \nabla T_\sigma) = \Omega(T_\sigma) \text{ at } A_{\beta\sigma}, \quad (3)$$

$$(\rho C_p)_\sigma \partial_t T_\sigma = \nabla \cdot (k_\sigma \nabla T_\sigma) + R_\sigma(T_\sigma) \text{ in } V_\sigma \quad (4)$$

This problem has to be solved together with the following total mass and momentum equations

$$\nabla \cdot \mathbf{v}_\beta = 0 \text{ in } V_\beta \quad (5)$$

$$\rho_\beta \mathbf{v}_\beta \cdot \nabla \mathbf{v}_\beta = -\nabla p_\beta + \rho_\beta \mathbf{g} + \mu_\beta \nabla^2 \mathbf{v}_\beta \text{ in } V_\beta \quad (6)$$

$$\mathbf{v}_\beta = 0 \text{ on } A_{\beta\sigma} \quad (7)$$

In this paper, the assumption is made that density and viscosity do not vary with temperature. Therefore, equations 5 through 7 may be solved independently from the heat transfer problem.

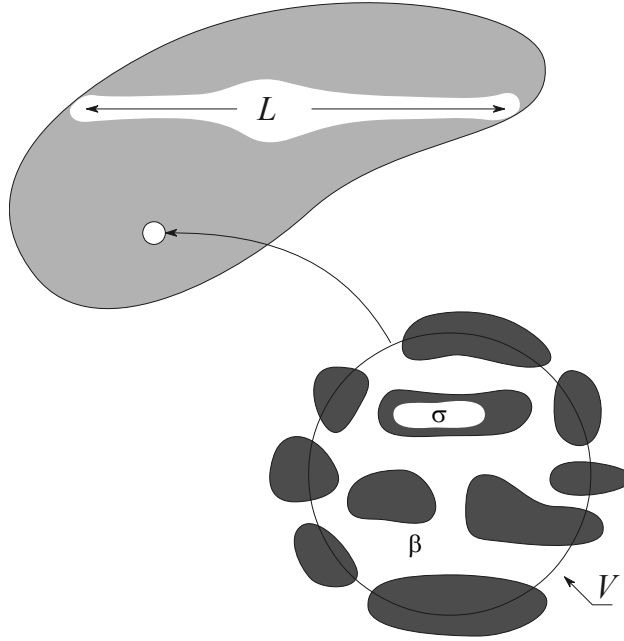


Figure 1 : Titre de la figure

The upscaling of the heat transfer problem has received a lot of attention in the literature. It is emphasized in [1] that several models may be developed:

- direct numerical simulation and heuristic models [2, ...]
- one-temperature, local equilibrium models [3, 4, ...],
- two-temperature, local non-equilibrium models, with linear driving force [5, 6, ...] or more sophisticated mathematical expressions involving, for instance, convolution products [7, 8, ...],
- various one-temperature representations of non-equilibrium situations [9, 10, 11, ...], such as the asymptotic behavior of two-temperature models, fractional derivatives, wave equations [12], etc...
- hybrid or mixed models coupling macro-scale equations with micro-scale pore-scale submodels.

In this paper, we particularly discuss the way the heat sources appear in the macro-scale models. In the case of a local equilibrium model, a total source term is introduced in the equation for the mixture temperature,  $T^{\beta\sigma}$ , under the form

$$R^{\text{LE}} = \varepsilon_{\beta} R_{\beta} (T^{\beta\sigma}) + \varepsilon_{\sigma} R_{\sigma} (T^{\beta\sigma}) - a_v \Omega (T^{\beta\sigma}) \quad (8)$$

where  $a_v = A_{\beta\sigma}/V$  is the specific area of the porous medium. The macro-scale source term is simply the average of the pore-scale source terms. In the case of local non-equilibrium models, the homogeneous source terms, as far as non-linearities are not concerned, do not pose a problem and averages appear in the right-hand sides of the respective phase equations. This is another matter for the heterogeneous source term. In the engineering practice, for instance catalytic burners [13], the total produced heat flux is assigned to the solid phase. However, a thorough pore-scale analysis or upscaling results do not necessarily support this choice as it is emphasized in this paper.

The objective of this work is two-fold. First, following [1, 14], the theory that leads to a local non-equilibrium model incorporating the effect of the heat sources terms is briefly developed. Then some quantitative applications of the theory that emphasize the applicability of the proposed model are presented.

## 2. Theory

Averages are defined classically as [15]

$$\langle \psi_\beta \rangle = \frac{1}{V} \int_{V_\beta} \psi_\beta dV \quad (9)$$

for any variable  $\psi_\beta$  defined in the  $\beta$ -phase. The phase intrinsic average is defined as

$$\langle \psi_\beta \rangle = \varepsilon_\beta \langle \psi_\beta \rangle^\beta \quad (10)$$

with the  $\beta$ -phase volume fraction,  $\varepsilon_\beta$ , defined as

$$\varepsilon_\beta = \frac{1}{V} \int_{V_\beta} dV \quad (11)$$

Deviations to the averaged values are also classically defined as

$$\psi_\alpha = \langle \psi_\alpha \rangle^\alpha + \tilde{\psi}_\alpha \quad \alpha = \beta, \sigma \quad (12)$$

The mixture temperature,  $T^{\beta\sigma}$ , may now be defined precisely as

$$(\rho c_p)^* T^{\beta\sigma} = \varepsilon_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta + \varepsilon_\sigma (\rho c_p)_\sigma \langle T_\sigma \rangle^\sigma \quad (13)$$

with

$$(\rho c_p)^* = \varepsilon_\beta (\rho c_p)_\beta + \varepsilon_\sigma (\rho c_p)_\sigma \quad (14)$$

## 2.1. averaged equations and deviation equations

The upscaling theory is not described with all details in this paper, the reader is referred to the cited literature for an introduction to averaging, thermal dispersion, etc... Since the emphasis here is on heat sources, the appropriate references are taken from a first development given in [1] with a subsequent improvement in [14], especially in terms of a second order closure. Only major steps are outlined below.

The first step starts with the averaging of the pore-scale equations. Making use of the averaging theorems such as

$$\langle \nabla \psi_\beta \rangle = \nabla \langle \psi_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \psi_\beta dA \quad (15)$$

$$\langle \nabla \cdot \mathbf{A}_\beta \rangle = \nabla \cdot \langle \mathbf{A}_\beta \rangle + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \mathbf{A}_\beta dA \quad (16)$$

the averaging of Eq. 1 leads to

$$\underbrace{\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t}}_{\text{accumulation}} + \underbrace{\varepsilon_\beta (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle^\beta \cdot \nabla \langle T_\beta \rangle^\beta}_{\text{convection}} = \nabla \cdot \underbrace{\left[ k_\beta \left( \varepsilon_\beta \nabla \langle T_\beta \rangle^\beta + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) \right]}_{\text{conduction}} \quad (17)$$

$$- \underbrace{(\rho c_p)_\beta \nabla \cdot \langle \tilde{\mathbf{v}}_\beta \tilde{T}_\beta \rangle}_{\text{dispersion}} + \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla T_\beta dA}_{\text{interfacial flux}} + \langle R_\beta (\langle T_\beta \rangle^\beta + \tilde{T}_\beta) \rangle$$

A similar equation may be written for the  $\sigma$ -phase, i.e.,

$$\underbrace{\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t}}_{\text{accumulation}} = \nabla \cdot \underbrace{\left[ k_\sigma \left( \varepsilon_\sigma \nabla \langle T_\sigma \rangle^\sigma + \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\sigma\beta} \tilde{T}_\sigma dA \right) \right]}_{\text{conduction}} \quad (18)$$

$$+ \underbrace{\frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla T_\sigma dA}_{\text{interfacial flux}} + \langle R_\sigma (\langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma) \rangle$$

The temperature deviations are solutions of the pore-scale problem transformed using the decomposition Eq. 12 and subtracting the averaged equations. After some algebra, the governing equations for the deviations may be written as

$$\begin{aligned}
(\rho c_p)_\beta \frac{\partial \tilde{T}_\beta}{\partial t} + (\rho c_p)_\beta \tilde{\mathbf{v}}_\beta \cdot \nabla \langle T_\beta \rangle_\beta + (\rho c_p)_\beta \mathbf{v}_\beta \cdot \nabla \tilde{T}_\beta &= \nabla \cdot (k_\beta \nabla \tilde{T}_\beta) \\
- \varepsilon_\beta^{-1} \nabla \cdot \left( k_\beta \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \tilde{T}_\beta dA \right) - \varepsilon_\beta^{-1} k_\beta \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot \nabla \tilde{T}_\beta dA & \\
+ R_\beta \left( \langle T_\beta \rangle^\beta + \tilde{T}_\beta \right) - \left\langle R_\beta \left( \langle T_\beta \rangle^\beta + \tilde{T}_\beta \right) \right\rangle^\beta & \quad (19)
\end{aligned}$$

$$\text{BC1} \quad \tilde{T}_\beta = \tilde{T}_\sigma - \underbrace{\left( \langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right)}_{\text{source term}} \quad \text{at } A_{\beta\sigma} \quad (20)$$

$$\begin{aligned}
\text{BC2} \quad - \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \tilde{T}_\beta - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla \langle T_\beta \rangle^\beta}_{\text{source term}} &= - \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \tilde{T}_\sigma - \underbrace{\mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla \langle T_\sigma \rangle^\sigma}_{\text{source term}} \\
+ \Omega \left( \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma \right) & \quad \text{at } A_{\beta\sigma} \quad (21) \\
\underbrace{\hspace{10em}}_{\text{source term}}
\end{aligned}$$

$$\begin{aligned}
(\rho c_p)_\sigma \frac{\partial \tilde{T}_\sigma}{\partial t} &= \nabla \cdot (k_\sigma \nabla \tilde{T}_\sigma) - \varepsilon_\sigma^{-1} \nabla \cdot \left( k_\sigma \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\sigma\beta} \tilde{T}_\sigma dA \right) \\
- \varepsilon_\sigma^{-1} k_\sigma \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\sigma\beta} \cdot \nabla \tilde{T}_\sigma dA + R_\sigma \left( \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma \right) - \left\langle R_\sigma \left( \langle T_\sigma \rangle^\sigma + \tilde{T}_\sigma \right) \right\rangle^\sigma & \quad (22) \\
\underbrace{\hspace{10em}}_{\text{source term}}
\end{aligned}$$

There are several source terms in these equations that will produce deviations of the temperature fields from the averaged values. A *closure* of the coupled macro-scale and micro-scale equations will require to find an approximate expression linking the deviations to the averaged values through the source terms. The source term in Eq. 20 and the first two ones in Eq. 21 will lead to classical thermal dispersion, tortuosity and interphase exchange effects, which have been dealt with at length in many papers (see for instance discussion in [1, 14, 15]). In this work, we focus on the impact of the heat source terms.

If the heat source terms are constant, as is the case for instance in nuclear safety problems where they are produced by radioactivity, the homogeneous source terms in the bulk equations for the deviations disappear and do not play longer a role in the closure problem while the heterogeneous term in BC2 remains. Developing the source term by a Taylor's expansion around the averaged temperature, one obtains

$$R_\alpha (T_\alpha) = R_\alpha (\langle T_\alpha \rangle^\alpha) + \left. \frac{\partial R_\alpha}{\partial T} \right|_{\langle T_\alpha \rangle^\alpha} \tilde{T}_\alpha + \dots \quad (23)$$

In this work, we will assume that the deviation part in Eq. 23 is small compared to  $R_\alpha (\langle T_\alpha \rangle^\alpha)$ . The validity of such an assumption will depend on the process under consideration. An example can be found in [16] in the case of source terms produced by an Arrhenius reaction rate. In this reference, it is shown that the above assumption works relatively well as soon as some Damköhler number remains small. Significant discrepancies arise otherwise. Neglecting higher order terms in Eq. 23 leads to the following approximation

$$R_\alpha (T_\alpha) \simeq R_\alpha (\langle T_\alpha \rangle^\alpha) \quad \text{and} \quad \Omega (T_\sigma) \simeq \Omega (\langle T_\sigma \rangle^\sigma) \quad (24)$$

which is used in the further developments.

As a consequence, the only remaining source term in the closure problem due to the heat sources is the one associated to the heterogeneous source term.

## 2.2. closure and macro-scale equations

It is beyond the scope of this paper to discuss the various models (transient closure, hybrid models, quasi-steady closure, asymptotic models, etc...) that can be developed from the averaged and deviation equations as discussed in [14]. Following [1, 14], a quasi-steady closure (closure is intended here as an approximate solution of the coupled macro and micro-scale equations), can be developed under the following form

$$\begin{aligned} \tilde{T}_\beta &= \mathbf{b}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma - s_\beta \left( \langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + r_\beta \Omega \\ &\quad + \mathbf{W}_{\beta\beta} \cdot \nabla \nabla \langle T_\beta \rangle^\beta + \mathbf{W}_{\beta\sigma} \cdot \nabla \nabla \langle T_\sigma \rangle^\sigma + \dots \end{aligned} \quad (25)$$

$$\begin{aligned} \tilde{T}_\sigma &= \mathbf{b}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{b}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma + s_\sigma \left( \langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + r_\sigma \Omega \\ &\quad + \mathbf{W}_{\sigma\beta} \cdot \nabla \nabla \langle T_\beta \rangle^\beta + \mathbf{W}_{\sigma\sigma} \cdot \nabla \nabla \langle T_\sigma \rangle^\sigma + \dots \end{aligned} \quad (26)$$

where second order terms have been kept. The mapping variables, i.e.,  $\mathbf{b}_{\beta\beta}$ ,  $\mathbf{b}_{\beta\sigma}$ , etc..., obey governing equations which realize an approximate solution of the coupled macro micro-scale system of equation. The first three terms in Eqs. 25 and 26 corresponds to the classical theory for the first order two-temperature model and will not be discussed here. The reader can refer to [6] for resolution of the three corresponding closure problems and calculations of the related effective properties, i.e., thermal dispersion tensors, heat exchange coefficient, etc... The other terms are not “traditional” and represent the contribution of the heterogeneous source, which will be discussed later, and of second order terms.

The resulting macro-scale equations are obtained by substituting Eqs. 25 and 26 into Eqs. 17 and 18. One obtains

$$\begin{aligned} \varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} + (\rho c_p)_\beta \langle \mathbf{v}_\beta \rangle \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\beta\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \\ \nabla \cdot \left( \mathbf{K}_{\beta\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\beta\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) - h_{2eq} \left( \langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) \\ + a_v \xi \Omega \left( \langle T_\sigma \rangle^\sigma \right) + \varepsilon_\beta R_\beta \left( \langle T_\beta \rangle^\beta \right) \end{aligned} \quad (27)$$

$$\begin{aligned} \varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} - \mathbf{u}_{\sigma\beta} \cdot \nabla \langle T_\beta \rangle^\beta - \mathbf{u}_{\sigma\sigma} \cdot \nabla \langle T_\sigma \rangle^\sigma = \nabla \cdot \left( \mathbf{K}_{\sigma\beta}^* \cdot \nabla \langle T_\beta \rangle^\beta + \mathbf{K}_{\sigma\sigma}^* \cdot \nabla \langle T_\sigma \rangle^\sigma \right) \\ - h_{2eq} \left( \langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + a_v (1 - \xi) \Omega \left( \langle T_\sigma \rangle^\sigma \right) + \varepsilon_\sigma R_\sigma \left( \langle T_\sigma \rangle^\sigma \right) \end{aligned} \quad (28)$$

In these macro-scale equations, the effective parameters are calculated from the mapping variables. For instance, the exchange coefficient is expressed as

$$h_{2eq} = \frac{1}{V} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla s_\beta dA \quad (29)$$

The macro-scale terms associated to the homogeneous heat source terms are simply the pore-scale function calculated at the average temperature weighted by the phase volume fraction. This is a consequence of neglecting high non-linearities as shown in Eq. 23. On the contrary, the heterogeneous heat source term is not entirely affected to a particular phase equation but, instead, has to be distributed between the two phase macro-scale equations. This is achieved through the introduction of a distribution coefficient which can be calculated from the pore-scale properties by solving the following closure problem:

$$\rho_\beta c_{p\beta} \mathbf{v}_\beta \cdot \nabla r_\beta = k_\beta \nabla^2 r_\beta - a_v \varepsilon_\beta^{-1} \xi_\beta, \quad \text{in } V_\beta \quad (30)$$

$$\text{BC1} \quad \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla r_\beta = \mathbf{n}_{\beta\sigma} \cdot k_\sigma \nabla r_\sigma + 1, \quad \text{at } A_{\beta\sigma} \quad (31)$$

$$\text{BC2} \quad r_\beta = r_\sigma, \quad \text{at } A_{\beta\sigma} \quad (32)$$

$$0 = k_\sigma \nabla^2 r_\sigma - a_v \varepsilon_\sigma^{-1} \xi_\sigma, \quad \text{in } V_\sigma \quad (33)$$

$$r_\beta(\mathbf{r} + \ell_i) = r_\beta(\mathbf{r}), \quad r_\sigma(\mathbf{r} + \ell_i) = r_\sigma(\mathbf{r}), \quad i=1,2,3 \quad (34)$$

$$\langle r_\beta \rangle^\beta = 0, \quad \langle r_\sigma \rangle^\sigma = 0 \quad (35)$$

where the distribution coefficient  $\xi$  is given by

$$\xi = \xi_\beta = \frac{1}{A_{\beta\sigma}} \int_{A_{\beta\sigma}} \mathbf{n}_{\beta\sigma} \cdot k_\beta \nabla r_\beta dA, \quad \xi_\sigma = 1 - \xi_\beta = \frac{1}{A_{\sigma\beta}} \int_{A_{\sigma\beta}} \mathbf{n}_{\sigma\beta} \cdot k_\sigma \nabla r_\sigma dA \quad (36)$$

In the next section, some properties of this distribution coefficient are discussed.

### 3. Applications: the distribution coefficient

In this section, the closure problem for the heterogeneous heat source term is solved for various pore-scale geometry and physical parameters. Then, a 0D macro-scale problem is solved to emphasize some peculiar features of this heat distribution problem.

#### 3.1. Results for the distribution coefficient

The closure problem expressed by Eqs. 30 through 36 has been solved analytically for stratified unit cells and 2D ou 3D simple unit cells[14]. In this paper, results are presented for a more realistic porous medium obtained from x-ray tomography [1].

In the case of a stratified unit cell such as the one represented Figure 2a, the distribution coefficient can be obtained analytically. Its value does not depend on the velocity and is given by

$$\xi = \frac{\varepsilon_\sigma k_\beta}{\varepsilon_\sigma k_\beta + \varepsilon_\beta k_\sigma} \quad (37)$$

An example of calculation of the distribution coefficient in the case of more complex unit cells is provided below. The pore-scale geometry is taken from an X-ray microtomograph and the solid phase indicator is represented Figure 2b.

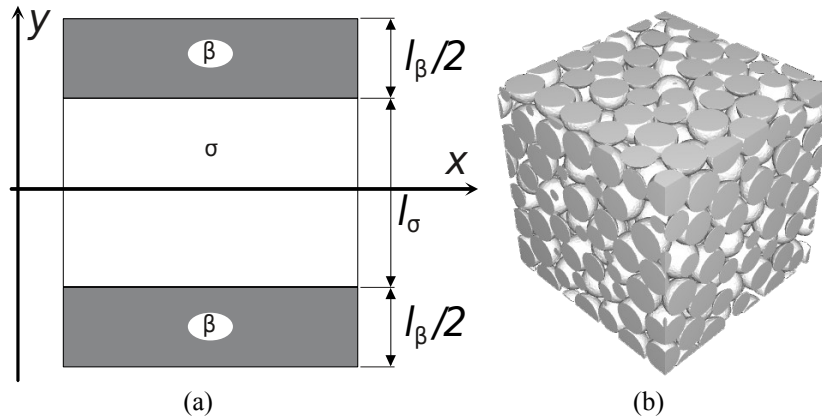


Figure 2. Unit Cells (UC)

The evolution of the distribution coefficient as a function of the thermal conductivity ratio is provided Figure 3 for three different unit cells (UC). They all have the same general trend:

$$\lim_{k_r \rightarrow -\infty} \xi = 1 \quad ; \quad \lim_{k_r \rightarrow \infty} \xi = 0 \quad \text{with } k_r = k_\sigma/k_\beta \quad (38)$$

In other words, the heterogeneous heat source has the tendency to be distributed towards the most conductive phase. If the practical problem under consideration involves a highly conductive solid phase, which is the case for instance in metallic catalytic porous burners, the heat source is affected to the  $\sigma$ -phase equation, which is the *common engineering practice*. In between these two limits, the detailed variation depends on the pore-scale geometry. The results emphasize the fact that the resulting distribution coefficient value is very sensitive to the pore-scale geometry and cannot be predicted accurately from results for simple unit cells.

The impact of the velocity field has been studied in [14]. Results for simple 2D unit cells are provided Figure 4. The Péclet number is defined as

$$\text{Pe} = \frac{(\rho c_p)_\beta \langle v_\beta \rangle^\beta l_c}{k_\beta} \quad (39)$$

where  $l_c$  is the array unit vector length (very close here to the grain diameter). The results show a transition regime for  $Pe$  between 1 and 100 in between two constants for  $Pe \rightarrow 0$  and  $Pe \rightarrow \infty$ . In the range of explored values, the distribution coefficient varies between 10 to 20%, which is less significant than the influence of the thermal conductivity ratio.

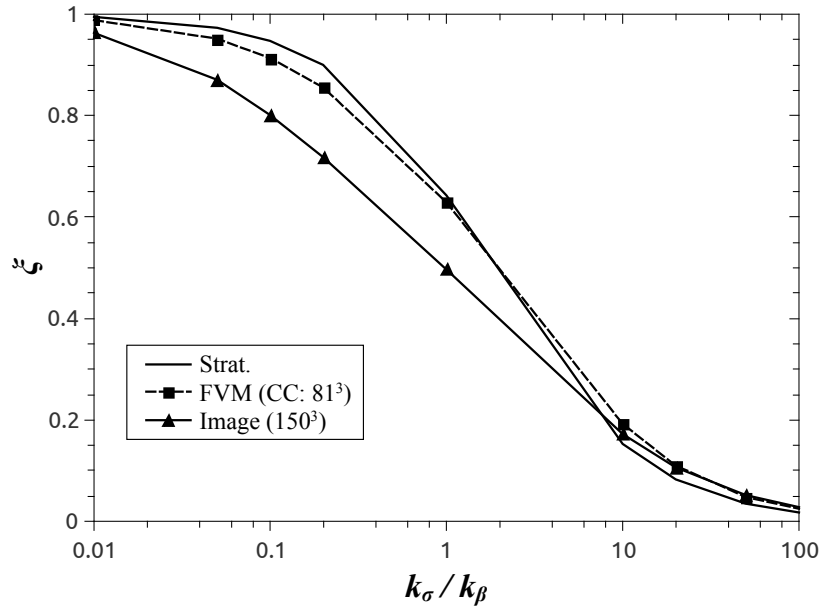


Figure 3. Distribution coefficient as a function of  $k_\sigma/k_\beta$  (Strat.=stratified UC; FVM=Cubic Centered; Image=X-ray tomography)

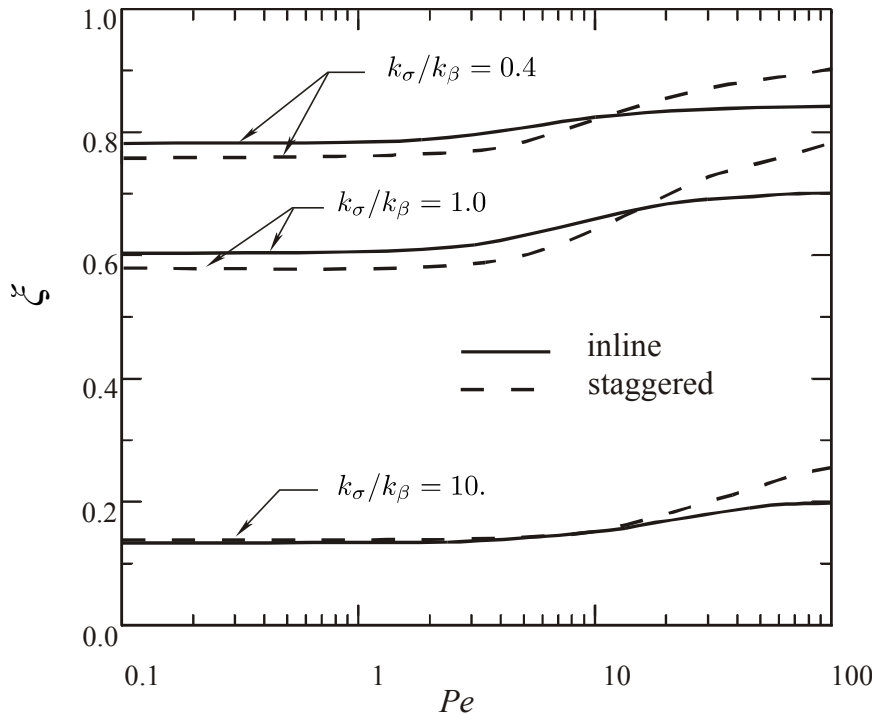


Figure 4. Distribution coefficient as a function of the Péclet number for two types of arrays of cylinders and various values of the thermal conductivity ratio.

### 3.2. Influence of the distribution coefficient on the temperature difference

Another common sense view of the problem is that the hottest phase, macroscopically speaking, is the one with the larger diffusivity. Let us explore that notion by looking at the following macro-scale 0D problem.

$$\varepsilon_\beta (\rho c_p)_\beta \frac{\partial \langle T_\beta \rangle^\beta}{\partial t} = -h_{2eq} \left( \langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) + a_v \xi \Omega \quad (40)$$

$$\varepsilon_\sigma (\rho c_p)_\sigma \frac{\partial \langle T_\sigma \rangle^\sigma}{\partial t} = -h_{2eq} \left( \langle T_\sigma \rangle^\sigma - \langle T_\beta \rangle^\beta \right) + a_v (1 - \xi) \Omega \quad (41)$$

$$\text{IC} \quad \langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = 0 \quad (42)$$

Solving analytically this problem, it can be shown that, after a transient behavior, the two macro-scale temperatures increase with time but the temperature difference is constant and given by

$$\lim_{t \rightarrow \infty} \left( \langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma \right) = \frac{\xi \varepsilon_\sigma (\rho c_p)_\sigma - (1 - \xi) \varepsilon_\beta (\rho c_p)_\beta}{h_{2eq} \left( \varepsilon_\sigma (\rho c_p)_\sigma + \varepsilon_\beta (\rho c_p)_\beta \right)} a_v \Omega \quad (43)$$

and the condition for obtaining a zero difference is

$$\xi = \frac{\varepsilon_\beta (\rho c_p)_\beta}{\varepsilon_\sigma (\rho c_p)_\sigma + \varepsilon_\beta (\rho c_p)_\beta} \quad (44)$$

In order to better understand the implications, let us consider the case of the stratified material represented Figure 2. Solving analytically the closure problem in that case gives

$$\frac{h_{2eq} (l_\beta + l_\sigma)^2}{k_\beta} = \frac{12 \left( \frac{k_\sigma}{k_\beta} \right)}{\varepsilon_\sigma + \varepsilon_\beta \frac{k_\sigma}{k_\beta}} \quad (45)$$

and

$$\xi = \frac{\varepsilon_\sigma k_\beta}{\varepsilon_\sigma k_\beta + \varepsilon_\beta k_\sigma} \quad (46)$$

The condition Eq. 44 gives

$$\langle T_\beta \rangle^\beta - \langle T_\sigma \rangle^\sigma = 0 \Rightarrow \frac{k_\sigma}{\varepsilon_\sigma^2 (\rho c_p)_\sigma} = \frac{k_\beta}{\varepsilon_\beta^2 (\rho c_p)_\beta} \quad (47)$$

We see that, if the volume fractions are the same, the change in the sign of the temperature difference occurs indeed when the diffusivities are equal. However, this is no longer true for different volume fractions. In fact, the material with the lowest diffusivity can have a higher averaged temperature if it is thin enough to catch up with the thicker phase! This is another feature, apparently counter intuitive, of this heterogeneous heat source problem.

## Conclusion

The introduction of heat source terms in macro-scale equations in the case of local non-equilibrium models requires the resolution of more complex closures. An example is provided in this paper in the case of a quasi-steady closure which generally leads to the classical two-temperature model. This model is modified here with the introduction of a distribution coefficient which insert a portion of the heterogeneous heat source into the each macro-scale phase equation. This coefficient varies rapidly for thermal conductivity ratios between 0.01 and 100, and the value is relatively sensitive to the pore-scale geometry as emphasized by the calculations on simple unit cells and also on a tomographic image.

This concept has already been used in various contexts: for instance for heat sources coming from Arrhenius reactions [16], for a local non-equilibrium heat transfer model including radiative heat transfer [17]. It proved very useful, which suggests that improvements should be sought in various different directions: higher order closures for non-linear systems, multi-physic coupling, etc...



## Nomenclature

Symbol	Name, <i>unit</i>		
$c_p$	heat capacity, J/kg.K	$\alpha$	refers to $\alpha$ -phase
$g$	gravitational acceleration, m/s <sup>2</sup>	$\varepsilon$	volume fraction
$k$	thermal conductivity, W/m.K	$\mu$	dynamic viscosity, N.s/m <sup>2</sup>
$K$	effective thermal dispersion, W/m.K	$\zeta$	distribution coefficient
$T$	temperature, K	$\rho$	density, kg/m <sup>3</sup>
$a_v$	specific area, m <sup>-1</sup>	$\Omega$	heterogeneous heat source, J/m <sup>2</sup> .s
$v$	velocity, m/s		
$V$	averaging volume, m <sup>3</sup>	Indices	
$R$	homogeneous heat source, J/m <sup>3</sup> .s	eq	equilibrium
		$\beta\sigma$	mixture variable

## Greek Symbols

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