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CHAPTER 2

Modeling of Transfers at a Fluid-Porous Interface: A Multi-Scale Approach

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Abstract: Free flows above porous medium are present in many industrial or environmental applications. To study such problems, a common approach consists of coupling a free fluid model with a porous model, the transfers that occur at the fluid-porous interface being modeled through appropriate boundary conditions. However, the determination of these boundary conditions is not trivial and remains an important issue for the study of practical applications. Here, we present a multi-scale method that allows to determine the form of the boundary conditions and the value of the jump parameters that appear in the expression of these boundary conditions. This theoretical approach allows to analyze the physical nature of the jump coefficients, to understand the importance of the interface location and to determine whether these jump coefficients are intrinsic parameters or not.

Keywords: Darcy-Brinkman model, diffusive mass transfer, fluid-porous interface, Forchheimer model, interface location, intrinsic parameters, jump parameters, Kelvin-Helmholtz instability, multi-scale method, Stokes model, transition region, up-scaling tools.

1. INTRODUCTION

Many environmental or industrial applications involve flows in configurations where both free and permeable regions are present: turbulent flows above forest or urban areas, flows above gravel streambeds, flows in heat exchangers, in nuclear waste repositories, or in nuclear reactor vessel. To study such applications, a commonly used modeling approach is to consider two homogeneous regions – a free region and a porous one – separated by a discontinuous interface. In the free region, classical models are used whereas in the porous region, dedicated porous models are implemented depending on the studied phenomena: Darcy, Forchheimer or Darcy-Brinkman models for the fluid mechanic; effective conducto-convective models for the heat transfers; effective diffusive-reactive transport models for mass transport;...etc. To perform the study in the whole domain and to determine and quantify the role of the interface region, one need to connect the transport models used in each regions using appropriate boundary conditions.

Given the models used in each region, the question regarding the general form of the boundary conditions can be first looked at from a mathematical

view point. For example, to connect the Stokes and the Darcy-Brinkman models, since the equations are both of second order, one solution is to specify a condition on the velocity and a condition on the normal stress at the interface to close the problem in the whole domain. The simplest solution is to impose continuity of these two quantities as performed by Neale and Nader [18]. In a similar way, to connect diffusive mass transfer models at a fluid-porous interface, one solution is to specify a condition on the concentration and a condition on the normal mass flux at the interface, cf. Valdés-Parada *et al.* [28]. However, are other boundary conditions admissible from a mathematical view point? Furthermore, when the models used in each regions are not of the same order – Darcy and Stokes for example – or not of the same complexity -two-temperature versus one-temperature conducto-convective models for the heat transfers-, is it possible to a priori know which boundary conditions are admissible mathematically?

From a physical view point, other difficulties arise. A first difficulty regards the physic of the interfacial region. Are the physical phenomena in this transition region particular? Are their impacts on the overall flow and transfers crucial? For example, regarding conductive heat transfers in a fluid-porous region, the transfers in the transition region are not very specific and it is possible to account for

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them through an effective conductivity, that varies smoothly in the interfacial region [21]. On the contrary, regarding turbulent flows above a permeable wall, it can be shown that in the interfacial region, the mass and momentum transfers are highly enhanced due to the presence of a Kelvin-Helmholtz type of instability [4] and it is not straightforward to determine if specific models have to be added or not to account for this phenomena, cf. Chandesris and Jamet [7].

Once the transfers are characterized in the interfacial region, another difficulty regards the modeling of these transfers using homogeneous models and appropriate boundary conditions. How to determine the appropriate boundary conditions? Using which criteria? Indeed, the use of homogeneous models (i.e. models dedicated and valid in homogeneous regions) in the interfacial region where they are a priori not valid because the physical phenomena would be better represented using models dedicated to this specific region, greatly constrains the type of solutions that can be captured by the final model. Furthermore, it appears that, for given physical phenomena, the exact location of the interface inside the fluid-porous interfacial region can have an important impact on the obtained result [16, 17, 24] and not for other ones, see Prat [21].

To dissociate these two modeling difficulties which are associated to the physical modeling specific of the transfers in the interfacial region for the first one and to the use of a discontinuous model to represent them for the second one, our idea is to introduce three different levels of description of the fluid/porous transition and thus two up-scaling steps to determine appropriate boundary conditions at a fluid-porous interface.

In this paper, we focus on the determination of the appropriate boundary conditions at a discontinuous fluid-porous interface from a modeling view point. In section 2, we present a two-step approach based on three different levels of description of the interface. In this approach, the physical transfers in the fluid-porous transition region are first characterized and then, in a second step, a discontinuous model is introduced. This approach allows to understand the importance of the interface location as illustrated in section 3 where different up-scaling tools are presented on a mass transfer problem. Given these results, it is possible to analyze the physical nature of the jump coefficients, to determine whether these jump coefficients are intrinsic parameters or not (See section 4) and to analyze the specificities of discontinuous models at a fluid-porous interface.

2. A TWO-STEP APPROACH

In the study of Beavers and Joseph [2] of a laminar flow over a porous medium, the momentum transport in the free fluid region is described by the Stokes equations, while the Darcy's law is used in the porous medium. To connect the models used in each region while accounting for the enhancement of the fluid flow in the channel due to the presence of the porous medium, Beavers and Joseph introduce an empirical slip-boundary condition that relates the velocity gradient in the free-fluid to the slip velocity at the interface and to the Darcy velocity inside the porous medium (U_D)

$$\frac{du}{dy}\Big|_{0^+} = \frac{\alpha}{\sqrt{K_p}}(u - U_D), \qquad (1)$$

where y is the direction normal to the interface, u is the x-component of the average velocity in the free fluid, K_p is the permeability of the porous medium and α is a slip parameter. The origin of the y-coordinate is taken at the boundary of the porous medium. Using this semi-empirical relation, they are able to describe the observed enhancement of the fluid flow by adjusting the value of the slip parameter α.

To take into account the same effect, but using the Darcy-Brinkman model in the porous medium, Ochoa-Tapia and Whitaker [19] introduce the following momentum jump condition:

$$\frac{du}{dy}\Big|_{0^+} - \frac{1}{\phi_p}\frac{du}{dy}\Big|_{0^-} = \frac{\beta}{\sqrt{K_p}}u, \qquad (2)$$

where ϕ_p is the porosity of the porous medium and β is a dimensionless parameter, while assuming the continuity of the velocity.

In these two relations, α and β are dimensionless parameters, which are supposed to depend only upon the geometry of the transition region. They are considered or though of as intrinsic interfacial properties which characterize the momentum transfers at the interface. Furthermore, it should be pointed out that the two relations (1) and (2) suppose that the position of the interface is defined without ambiguity. However, at the pore scale, the transition between the homogeneous region and the free fluid region is not that sharp, in particular for most natural media, as illustrated in Fig. (**1**). In the same time, while focusing on the determination of the parameters α and β, various contributions [16, 25, 10] have shown that these parameters are not intrinsic and depend strongly on the choice, made during the modeling, of where to locate the interface inside the

transition region. This observation tends to reconsider the interpretation of these jump parameters as interfacial properties, specific of the transfers at the interface.
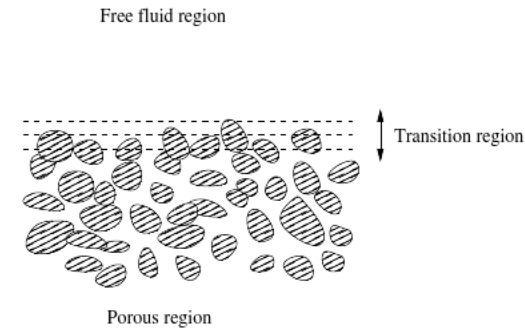
Free fluid region

Porous region

Fig. (**1**): Localization of the interface at the boundary of a porous medium. Different positions can be chosen inside the transition region.

The determination of these jump parameters values is crucial for many applications since these values characterize the transfers at the interface. The observation of a great sensitivity of the obtained values, to a parameter, the location of the interface, that is difficult to specify unambiguously has motivated the following two-step approach. Our idea is to dissociate in the modeling process what is related to the physics of the transfer in the fluid-porous transition region from what is related to the *choice* of modeling these transfers using homogeneous models and a discontinuous interface. For that, we introduce three different scales of description of the interface, as illustrated in Fig. (**2**).

2.1. Different Descriptions of a Fluid/Porous Transition

At the *microscopic* scale, where each pores of the porous medium are described, the transfers can be described in the whole domain by transport equations in the fluid and in the solid. Yet, in the porous region, such a description is not relevant. Indeed, first it is not always possible to describe exactly the geometry at the microscopic scale and second it might not be possible and it is certainly not pertinent to solve the problem at this scale. For these reasons, macroscopic equivalent models are used in the porous region, while the fluid transport equations are kept in the free fluid region.

Now, at the pore scale, the distinction between the homogeneous region and the free fluid one is not that clear, as illustrated in Fig. (**1**), and thus it is difficult to a priori state in a discontinuous description where the porous region ends. Furthermore, in the fluid-porous transition region, the transfers might be different from both the transfers in the porous and in the free fluid regions. For example, recirculations initiated by the presence of the solid grains can develop in the free part of the transition region. To take into account these two points, an approach consists in introducing a continuous level of description of the fluid-porous interface, denoted here the *mesoscopic* scale. At this continuous level, the zone located in between the two homogeneous regions is a continuous heterogeneous region. In this transition region, the properties of the medium are supposed to encounter strong but nevertheless continuous variations. Thus, the porosity varies continuously between the two regions. This approach allows to skip the question relative to the location of the interface while modeling the porous region. One does not need to specify where the porous region ends. Regarding the other medium properties (permeability, effective conductivity or diffusivity), their continuous variations allows to describe the continuous variations of the transfers in this region and their possible specificities.

The macroscopic scale corresponds to a description where the interface is discontinuous and where the effective transport properties are constant on both side of the interface. Although the mesoscopic continuum description accounts for the underlying physic of the transfer in the transition region, the macroscopic level is generally more useful for the study of practical applications since it involves only constant effective properties. However, this means that the precision of the description is lowed down at this scale, especially in the transition region where constant instead of variable properties are used.

2.2. Modeling Transfers with Continuous Models

To derive models at the mesoscopic scale, one approach consists in applying the volume average, used to model the porous zone, not only in the porous region but in the entire domain and in particular across the interfacial region. After applying this averaging volume, closure relations must be specified to obtain the effective properties of the continuous medium. Unlike the case of homogeneous porous media where the closure relations can be proved under certain length-scale restrictions (Whitaker [31]), up to now, no formal approach ex-
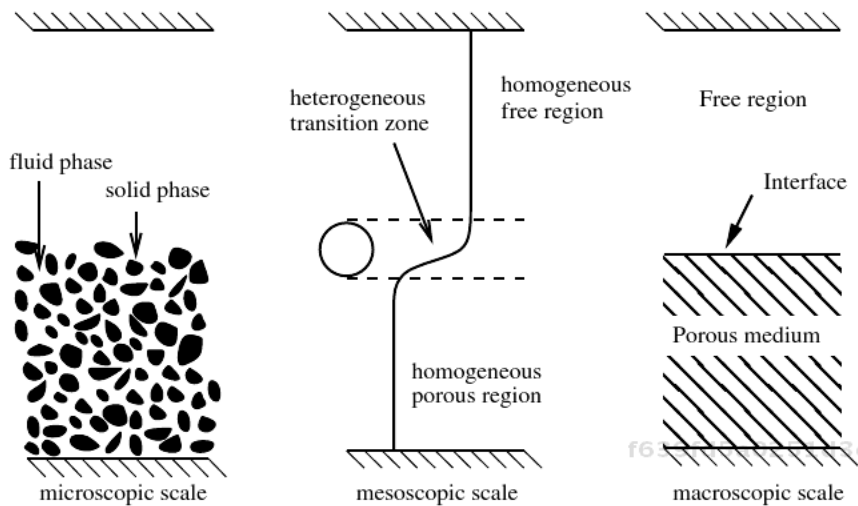
Fig. (**2**): The interface between a homogeneous porous medium and a free fluid region at different scales of description.

ists to derive such relations in the interfacial transition region. Indeed, the derivation of the closure problems in the homogeneous regions is based on a superposition principle which is proved to be valid under certain length-scale constraints. Its extension to the transition region, where these length-scale restrictions are not verified, is not straightforward even though it is the subject of ongoing research [29, 30].

Nevertheless, these closure relations can be postulated a priori and their validity can be checked a posteriori. For example, Saleh *et al.* [24] have shown, based on their experimental observations of a flow above a permeable media, that "*it seems necessary to take into account a variation of the permeability in an intermediate layer*" to describe the momentum transfers in the interfacial region. Postulating the validity of a variable permeability model in the transition region, the variation of the permeability can then be obtained from the velocity field of volume averaged microscopic numerical simulations [25, 3]. In the same way, for conductive or conducto-convective heat transfer problems, postulating the validity of a variable effective conductivity or diffusivity tensor, the variations of these tensors can then be deduced from the variations of the temperature field [8, 21, 26, 27].

At this continuous scale, the criteria to derive the transport models is to match the volume averaged velocity or temperature fields obtained by volume averaging microscopic simulations or experimental data with the solution of the model in the interfa-

cial region. Given this criteria based on averaged fields, and since the effective transport coefficients or properties are usually different in the homogeneous free fluid and porous regions, these various contributions show that the interfacial region must be viewed as a transition region for the effective transport coefficients or properties. The transfers in the interfacial region are different from those in each homogeneous regions and a solution to account for their specificities is to use continuous models. The physic of the transfers and of their potential specificities in the interfacial region is thus characterized at this scale and a continuous model is necessary.

It might be pointed out that one difficulty to derive these continuous models lies in the choice of their form. Indeed, since no formal approach exists to determine what is the form of the closure relations in the interfacial transition region, different choices can be made. For example, regarding the momentum transfer at a fluid-porous interface, different continuous models can be found in the literature for the transition region. The one used by Chandesris and Jamet [5]:

$$0 = -\nabla \langle p \rangle^f + \frac{\mu}{\phi(\mathbf{x})} \nabla \cdot \nabla \langle \mathbf{u} \rangle - \mu \, \mathbf{K}(\mathbf{x})^{-1} \cdot \langle \mathbf{u} \rangle \,, \quad (3)$$

where $\langle p \rangle^f$ is the intrinsic averaged pressure, $\langle \mathbf{u} \rangle$ is the volume averaged velocity, μ is the fluid viscosity, ϕ is the porosity and $\mathbf{K}$ is the permeability

tensor. The one suggested in Goyeau *et al.* [14]:

$$0 = -\nabla \langle p \rangle^f + \mu \nabla \cdot \left(\frac{1}{\phi(\mathbf{x})} \nabla \langle \mathbf{u} \rangle \right) - \mu \, \mathbf{K}(\mathbf{x})^{-1} \cdot \langle \mathbf{u} \rangle \tag{4}$$

or the one used in Valdès-Parada *et al.* [30]:

$$0 = -\nabla \langle p \rangle^f + \mu \nabla \cdot \left(\frac{1}{\phi(\mathbf{x})} \nabla \langle \mathbf{u} \rangle \right) \\ + \left(\frac{(\nabla \phi(\mathbf{x}))^2}{\phi(\mathbf{x})^3} - \mu \, \mathbf{K}(\mathbf{x})^{-1} \right) \cdot \langle \mathbf{u} \rangle . \tag{5}$$

These models are identical in the homogeneous regions ($\phi = $ const). The difference is very small and concerns the location of the variable porosity in the stress tensor. Depending on which model is chosen, different permeability profiles are obtained, even though these profiles are very close.

2.3. Modeling Transfers with Discontinuous Models

These mesoscopic continuous descriptions account for the underlying physic of the transfer in the transition region. However, the use of variable properties is not always relevant for the study of practical applications. Indeed, it requires first to precisely determine these variable properties and secondly to use a mesh adapted to these variations which can imply an important computational cost. Furthermore, the exact capture of the different fields in the interfacial transition region is not always necessary and the determination of the overall transfers is usually enough. For these reasons, a less detailed description, based on discontinuous models and boundary conditions at the interface, is often preferred. The difficulty is then to determine the appropriate boundary conditions and their associated coefficients, which traduce correctly the transfers of the transition region.

In the next section, we focus on this second up-scaling step, i.e. the mesoscopic-macroscopic up-scaling. Our goal is to show both theoretically and through an illustrative example, how a continuous model can be traduced into a discontinuous one and thus how to determine the associated boundary conditions.

3. FROM CONTINUOUS TO DISCONTINUOUS MODELS

This second up-scaling is performed to go from a continuous description of the interface to a discontinuous one. It has been thoroughly studied for two-phase systems such as liquid/liquid, liquid/vapor or liquid/solid interfaces [1, 12, 13]. Different theories and methods have been developed to study this kind of up-scaling. They have their benefits and drawbacks depending on the studied problem, as we will show in the following for two particular methods. However, one notion is always present in those methods: the notion of *surface-excess quantity*.

3.1. Surface-Excess Theory

To present the surface-excess theory and the associated general results, we consider the following diffusive-reactive mass transfer process that is supposed to be valid at the mesoscopic scale:

$$\phi(\mathbf{x}) \frac{\partial \langle c \rangle^f}{\partial t} = -\nabla \cdot q + k(\mathbf{x}) \langle c \rangle^f , \tag{6}$$

where q is the mass flux at the mesoscopic scale:

$$q = -\phi(\mathbf{x}) \mathbf{D}(\mathbf{x}) \cdot \nabla \langle c \rangle^f . \tag{7}$$

$\langle c \rangle^f$ is the intrinsic averaged mass fraction of a given species, ϕ is the porosity, $\mathbf{x}$ is the local co-ordinate, and $\mathbf{D}$ and k are respectively an effective diffusivity tensor and an effective reaction rate coefficient that vary in the interfacial transition region. Thus, the physic of the transfers and their potential specificities in the interfacial region are supposed to be characterized at this continuous scale through the variation of ϕ, $\mathbf{D}$ and k in the direction normal to the interface. The effective reaction rate is supposed to be null in the free fluid region.

At the macroscopic scale, constant effective properties are used in each region and the mass transfer process is governed by the following equations. In the free fluid region:

$$\frac{\partial \tilde{c}_l}{\partial t} = -\nabla \cdot \tilde{q}_l , \tag{8}$$

where $\tilde{q}_l$ is the mass flux at the macroscopic scale in the free fluid region:

$$\tilde{q}_l = -D_l \nabla \tilde{c}_l . \tag{9}$$

In the homogeneous porous region:

$$\phi_p \frac{\partial \tilde{c}_p}{\partial t} = -\nabla \cdot \tilde{q}_p + k_p \tilde{c}_p , \tag{10}$$

where $\tilde{q}_p$ is the mass flux at the macroscopic scale in the porous region:

$$\tilde{q}_p = -\phi_p \mathbf{D}_p \cdot \nabla \tilde{c}_p . \tag{11}$$

$\tilde{c}_l$ and $\tilde{c}_p$ represent the mass fraction at the macroscopic scale, D_l is the diffusivity in the free fluid

region and ϕ_p, $\mathbf{D}_p$ and k_p are the porosity, the effective diffusivity and the effective reaction rate in the porous region.

The continuous transition region of the mesoscopic scale, characterized by variable effective transport properties, is thus replaced at the macroscopic scale by a discontinuous interface with constant effective properties on both sides of the interface. By doing this, one looses the local information of the mesoscopic model about the local transfers that occur in the interfacial region. However, the idea is to keep the overall effects of what happens in the transition region. If the overall transfers are conserved during the up-scaling process, the mesoscopic and macroscopic solutions will not differ outside of the transition region. Nevertheless, one expects that the two solutions will be different inside the transition region since the local information of the continuous model is lost as illustrated in Fig. (**3**).
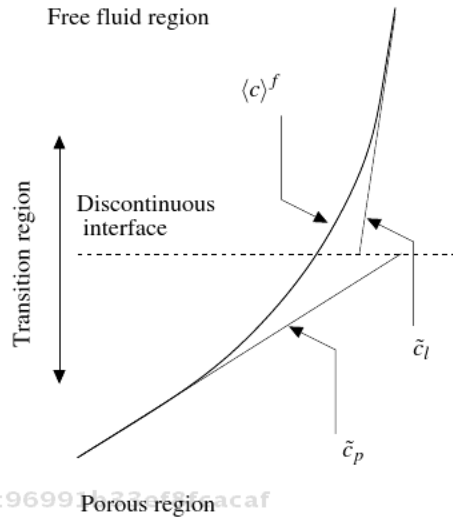

Fig. (**3**): Example of concentration profiles in the interfacial region at the meso- and macroscopic scales. The solutions do not differ outside of the transition region, but are different inside.

3.1.1. Flux Jump Condition

To ensure the conservation of the overall transfers in the interfacial transition region during the up-scaling process, the idea is to use a conservation principle [12]. Thus, one compares the integrals of the meso- and macroscopic conservation equations in the entire domain or at least in a region greater than the transition region as the volume V illustrated in Fig. (**4**).

Regarding the notation, the surface bounding the volume V is noted A. The volumes of the free fluid and porous regions contained in V are noted V_l and V_p. The surface A bounding the volume V is divided in two surfaces A_l and A_p located respectively in V_l and V_p. The surface separating the two regions is noted A_{lp}. To be clear, with these definitions, the surface bounding the volume V_l is the sum of the surface A_l and A_{lp}.
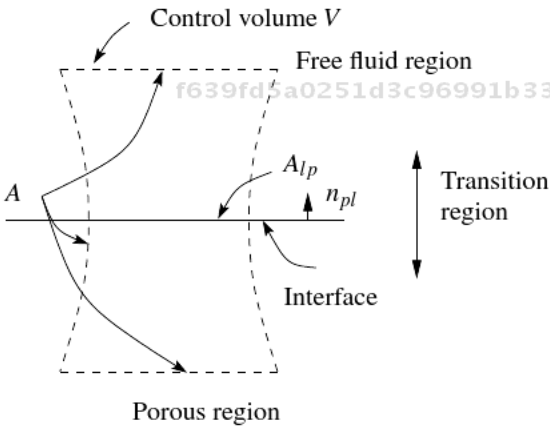

Fig. (**4**): Control volume surrounding the transition region.

We form the integral of equation (6) over V, the integrals of equation (8) and (10) over V_l and V_p respectively and substract the obtained results. One gets for the time derivative term, assuming that the porosity and the control volume V do not vary with time:

$$\int_V \phi(\mathbf{x})\frac{\partial \langle c\rangle^f}{\partial t}dV - \int_{V_l}\frac{\partial \tilde{c}_l}{\partial t}dV - \int_{V_p}\phi_p\frac{\partial \tilde{c}_p}{\partial t}dV = \frac{\partial}{\partial t}\left(\int_V \phi(\mathbf{x})\langle c\rangle^f dV - \int_{V_l}\tilde{c}_l dV - \int_{V_p}\phi_p\tilde{c}_p dV\right) \tag{12}$$

for the reaction term:

$$\int_V k(\mathbf{x})\langle c\rangle^f dV - \int_{V_p}k_p\tilde{c}_p dV \tag{13}$$

since the effective reaction rate is supposed to be null in the free fluid region. For the diffusion term,

the divergence theorem is used and one gets:

$$\int_V \nabla \cdot q\, dV - \int_{V_l} \nabla \cdot \tilde{q}_l\, dV - \int_{V_p} \nabla \cdot \tilde{q}_p\, dV =$$

$$\int_A \mathbf{n} \cdot q\, dA - \left(\int_{A_l} \mathbf{n}_l \cdot \tilde{q}_l\, dA + \int_{A_{lp}} \mathbf{n}_{lp} \cdot \tilde{q}_l\, dA \right)$$

$$- \left(\int_{A_p} \mathbf{n}_p \cdot \tilde{q}_p\, dA + \int_{A_{pl}} \mathbf{n}_{pl} \cdot \tilde{q}_p\, dA \right) =$$

$$+ \int_{A_{lp}} \mathbf{n}_{pl} \cdot (\tilde{q}_l - \tilde{q}_p)\, dA$$

$$+ \left(\int_A \mathbf{n} \cdot q\, dA - \int_{A_l} \mathbf{n}_l \cdot \tilde{q}_l\, dA - \int_{A_p} \mathbf{n}_p \cdot \tilde{q}_p\, dA \right), \tag{14}$$

where $\mathbf{n}$, $\mathbf{n}_l$ and $\mathbf{n}_p$ are the unit normal vectors associated respectively to the surface A, A_l and A_p. $\mathbf{n}_{lp}$ is the unit normal vector defined on the surface A_{lp} directed from the l-phase to the p-phase. With this convention, we have: $\mathbf{n}_{lp} = -\mathbf{n}_{pl}$.

Combining equations (12), (13) and (14), we have:

$$\int_{A_{lp}} \mathbf{n}_{pl} \cdot (\tilde{q}_l - \tilde{q}_p)\, dA =$$

$$- \frac{\partial}{\partial t} \left(\int_V \phi(\mathbf{x}) \langle c \rangle^f\, dV - \int_{V_l} \tilde{c}_l\, dV - \int_{V_p} \phi_p \tilde{c}_p\, dV \right)$$

$$+ \left(\int_V k(\mathbf{x}) \langle c \rangle^f\, dV - \int_{V_p} k_p \tilde{c}_p\, dV \right)$$

$$- \left(\int_A \mathbf{n} \cdot q\, dA - \int_{A_l} \mathbf{n}_l \cdot \tilde{q}_l\, dA - \int_{A_p} \mathbf{n}_p \cdot \tilde{q}_p\, dA \right). \tag{15}$$

The three terms under bracket appearing in the right-hand-side of equation (15) corresponds to surface-excess quantities.

A surface-excess quantity is a quantity per unit surface area assigned to the interface. For the general 3D case, it is defined as the integral of the difference between the mesoscopic and the macroscopic representations of this variable *in the direction normal to the interface*:

$$\psi^{ex} \triangleq \int_{\mathscr{L}} (\psi - \Psi)\, d\mathscr{L}, \tag{16}$$

where ψ is the mesoscopic representation of the studied field, Ψ is its macroscopic representation in the two homogeneous regions and $\mathscr{L}$ is a line element normal to the interface. The excess quantity is represented by the hatched area in Fig. (**5**). It represents exactly the amount of the ψ field that is not taken into account by the macroscopic model in the transition region compared to the mesoscopic model.
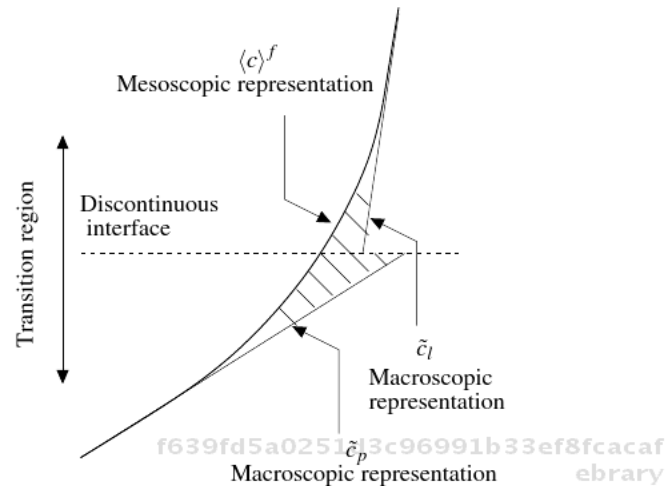

Fig. (**5**): Excess quantity.

When the size of the transition region is small compared to the characteristic macroscopic length scales, Edwards *et al.* [12] show that the following relations are verified. For a scalar quantity ψ:

$$\int_{A_{lp}} \psi^{ex}\, dA = \int_V (\psi - \Psi)\, dV$$

$$= \int_V \psi\, dV - \int_{V_l} \Psi_l\, dV - \int_{V_p} \Psi_p\, dV. \tag{17}$$

For a vector quantity ψ

$$\int_{\partial A_{lp}} \psi^{ex} \cdot d\mathbf{L} = \int_{\partial V} (\psi - \Psi) \cdot d\mathbf{A}$$

$$= \int_A \psi \cdot d\mathbf{A} - \int_{A_l} \Psi_l \cdot d\mathbf{A} - \int_{A_p} \Psi_p \cdot d\mathbf{A}, \tag{18}$$

where ∂A_{lp} is the contour of the surface A_{lp}. Furthermore, the divergence surface theorem gives:

$$\int_{\partial A_{lp}} \psi^{ex} \cdot d\mathbf{L} = \int_{A_{lp}} \nabla_s \cdot (\mathbf{I}_s \cdot \psi^{ex})\, dA, \tag{19}$$

where ∇_s is the surface divergence operator and $\mathbf{I}_s$ is the identity operator on the surface. Injecting these relations into equation (15), it comes:

$$\int_{A_{lp}} \mathbf{n}_{pl} \cdot (\tilde{q}_l - \tilde{q}_p)\, dA =$$

$$- \frac{\partial}{\partial t} \left(\int_{A_{lp}} \left(\phi \langle c \rangle^f \right)^{ex}\, dA \right) + \int_{A_{lp}} \left(k \langle c \rangle^f \right)^{ex}\, dA$$

$$- \int_{A_{lp}} \nabla_s \cdot (\mathbf{I}_s \cdot q^{ex})\, dA. \tag{20}$$

This relation being valid for any surface A_{lp}, one finally gets for any point $\mathbf{x}_M$ of the interface:

$$
\begin{aligned}
\mathbf{n}_{pl} \cdot [\tilde{q}_l - \tilde{q}_p]_{\mathbf{x}_M} = &-\frac{\partial}{\partial t}\left(\phi \langle c \rangle^f\right)^{ex} \\
&- \nabla_s \cdot (\mathbf{I}_s \cdot q^{ex}) + \left(k \langle c \rangle^f\right)^{ex}.
\end{aligned}
\tag{21}
$$

Mathematically, this equation is a boundary condition at the interface located at $\mathbf{x}_M$, that couples the solutions of the macroscopic problems $\tilde{c}_l$ and $\tilde{c}_p$ via their fluxes. The right-hand-side involves surface-excess quantities which correct the errors generated by the use of macroscopic models instead of the mesoscopic one inside the transition region. The jump condition (21) ensures that even though the mass fluxes are locally different inside the transition region between the meso- and macroscopic representations, their overall amount is the same if the balance is performed on a region that includes the transition region. For the overall transfers to be the same, one has to take into account, without any simplifications, a surface-excess accumulation term, which will be null for stationary problems, the surface divergence of a flux surface-excess, which will be null for one-dimensional problems and a surface-excess reaction term.

This approach is very general and can be applied to many kind of balance equations.

3.1.2. Concentration Jump Condition

To close the problem at the macroscopic scale, a boundary condition on the averaged concentration must also be specified. In various contributions [20, 28], the continuity of this quantity (or of the temperature if studying a heat transfer problem) is assumed. In fact, the boundary condition on the averaged concentration can also be deduced using the surface excess theory, starting from the relation between the mass flux and the concentration.

We form the integral over V of equation (7) divided by $\phi(\mathbf{x})\mathbf{D}(\mathbf{x})$, the integrals over V_l and V_p respectively of equation (9) divided by D_l and (11) divided by $\phi_p \mathbf{D}_p$ and substract the obtained results:

$$
\int_V \nabla \langle c \rangle^f \, dV - \int_{V_l} \nabla \tilde{c}_l \, dV - \int_{V_p} \nabla \tilde{c}_p \, dV =
$$
$$
-\int_V \frac{\mathbf{D}^{-1}}{\phi} \cdot q \, dV + \int_{V_l} \frac{1}{D_l} \tilde{q}_l \, dV + \int_{V_p} \frac{\mathbf{D}_p^{-1}}{\phi_p} \cdot \tilde{q}_p \, dV.
\tag{22}
$$

Regarding the left-hand side of equation (22) it

comes, using the divergence theorem:

$$
\begin{aligned}
&\int_V \nabla \langle c \rangle^f \, dV - \int_{V_l} \nabla \tilde{c}_l \, dV - \int_{V_p} \nabla \tilde{c}_p \, dV = \\
&\int_{A_{lp}} \mathbf{n}_{pl} (\tilde{c}_l - \tilde{c}_p) \, dA \\
&+ \left(\int_A \mathbf{n} \langle c \rangle^f \, dA - \int_{A_l} \mathbf{n}_l \tilde{c}_l \, dA - \int_{A_p} \mathbf{n}_p \tilde{c}_p \, dA \right).
\end{aligned}
\tag{23}
$$

Regarding the last term of equation (23), one has, using the definition of the excess quantity and the divergence surface theorem:

$$
\begin{aligned}
&\left(\int_A \mathbf{n} \langle c \rangle^f \, dA - \int_{A_l} \mathbf{n}_l \tilde{c}_l \, dA - \int_{A_p} \mathbf{n}_p \tilde{c}_p \, dA \right) = \\
&\int_{\partial A_{lp}} \left(\langle c \rangle^f\right)^{ex} d\mathbf{L} = \int_{A_{lp}} \nabla_s \cdot \left(\mathbf{I}_s \left(\langle c \rangle^f\right)^{ex}\right) dA.
\end{aligned}
\tag{24}
$$

Combining equations (22)–(24), one finally gets for any point $\mathbf{x}_M$ of the interface:

$$
\begin{aligned}
[\tilde{c}_l - \tilde{c}_p]_{\mathbf{x}_M} = &-\mathbf{n}_{pl} \cdot \nabla_s \cdot \left(\mathbf{I}_s \left(\langle c \rangle^f\right)^{ex}\right) \\
&- \mathbf{n}_{pl} \cdot \left(\frac{\mathbf{D}^{-1}}{\phi} \cdot q\right)^{ex}.
\end{aligned}
\tag{25}
$$

This result shows that, a priori, one should take into account a jump on the concentration. This jump depends on a surface divergence term, which will be null for one-dimensional problem and a surface-excess diffusion term. The origin of this last term is related to the excess of the flux time the diffusion resistance.

Thus, the generic approach of the surface-excess theory is very powerful. It allows to derive the needed boundary conditions for any kind of transport equations, even in the general three-dimensional case. Furthermore, it highlights the origin of the possible jumps. They are related to surface-excess of the different tranfer mechanisms. However, the boundary conditions (21) and (25) are not closed. Indeed, the surface-excess quantities that appear in these relations depend on the mesoscopic unknown $\langle c \rangle^f$ and q. Before studying this question in section 3.4. using a different method, we illustrate these first results on a simplified one-dimensional example in order to illustrate some properties of the surface-excess quantities.

3.2. Surface-Excess Quantities and Location of the Interface

In this section, we consider a simplified version of the reaction-diffusion equation (6) for which

the problem is one-dimensional, stationary and the source term is given a priori and not concentration dependent:

$$0 = \frac{d}{dy}\left(\phi(y)D(y)\frac{d\langle c\rangle^f}{dy}\right) + S(y). \qquad (26)$$

At the macroscopic scale, constant effective properties are used in each region and the one-dimensional mass transfer process is governed by the following equations. In the free fluid region:

$$0 = \frac{d}{dy}\left(D_l\frac{d\tilde{c}_l}{dy}\right) + S_l. \qquad (27)$$

In the homogeneous porous region:

$$0 = \frac{d}{dy}\left(\phi_p D_p\frac{d\tilde{c}_p}{dy}\right) + S_p. \qquad (28)$$

The results obtained in the previous section are simplified. The flux jump condition (21) reduces to:

$$\left[-D_l\frac{d\tilde{c}_l}{dy} + \phi_p D_p\frac{d\tilde{c}_p}{dy}\right]_{y_M} = S^{ex}, \qquad (29)$$

since here, $\mathbf{n}_{pl} = 1$, and the averaged concentration jump condition (25) reduces to:

$$[\tilde{c}_l - \tilde{c}_p]_{y_M} = -\left(\frac{q}{\phi D}\right)^{ex}. \qquad (30)$$

Since the source term is supposed to be given, for this very simplified 1D problem, the mass flux q is also given at a constant. It is not an unknown of the problem. Thus, given the profile of the porosity $\phi(y)$, the effective diffusivity $D(y)$ and the source term $S(y)$, one can compute the surface-excess quantities involved in the two boundary conditions using the definition (16) of an excess quantity. For a one-dimensional problem, this equation can be rewritten:

$$\psi^{ex} = \int_{-\infty}^{y_M}(\psi(y)-\Psi^-)\,dy + \int_{y_M}^{+\infty}(\psi(y)-\Psi^+)\,dy. \qquad (31)$$

Given the definition (31) of a surface-excess quantity, it follows that its value depends on y_M when $\Psi^- \neq \Psi^+$. To illustrate this, a particular position y_ψ is introduced for which the sum of the two integral terms of equation (31) is zero:

$$\int_{-\infty}^{y_\psi}(\psi(y)-\Psi^-)\,dy + \int_{y_\psi}^{+\infty}(\psi(y)-\Psi^+)\,dy = 0. \qquad (32)$$

This particular position y_ψ is named the *center of gravity* of the profile of ψ. Using this definition, one gets, when Ψ^- and Ψ^+ are constants:

$$\psi^{ex} = (y_\psi - y_M)(\Psi^- - \Psi^+), \qquad (33)$$

which shows that, when Ψ^- and Ψ^+ are constants, the excess quantity depends linearly on y_M. Thus, when $\Psi^- \neq \Psi^+$, which is often the case when studying fluid-porous problem, the value of the excess quantities does depend on the location of the interface inside the transition region.

Nevertheless, this dependence of the excess quantity and thus of the jump coefficient, on the location of the interface, compensates the fact that the macroscopic problems are different in the two homogeneous regions ($\Psi^- \neq \Psi^+$). Thus, changing the interface location, modifies the zone of influence of a given macroscopic model. Finally, the value of the excess quantity is such that, whatever the location of the discontinuous interface inside the transition region, the overall amount of a given quantity is conserved at the macroscopic scale *via* its two asymptotic values in the homogeneous regions and *via* its excess quantity assigned to the interface.

When $\Psi^- = \Psi^+$, the value of the excess quantity do not depend on the interface location, since it can be rewritten:

$$\psi^{ex} = \int_{-\infty}^{+\infty}(\psi(y)-\Psi^-)\,dy. \qquad (34)$$

At the same time, since the macroscopic problems are equal in the two homogeneous regions ($\Psi^- = \Psi^+$), changing the interface location, do not modify the zone of influence of a given macroscopic model, since they are the same. Thus, in this case also, the value of the excess quantity is such that, whatever the location of the discontinuous interface inside the transition region, the overall amount of a given quantity is conserved at the macroscopic scale *via* the two asymptotic values of this quantity in the homogeneous regions and *via* the excess quantity assigned at the interface.

We illustrate these results using the two following source terms in the case where both the porosity and the diffusivity are constant (equal to one for simplicity). At the boundaries of the domain, we impose $c(-H) = c(H) = 0$.

3.2.1. A Simple Source Term

We consider first the following source term illustrated in Fig. (**6**)(a):

$$S_1(y) = S_p\left(\frac{-1}{2}\tanh\left(\frac{y-y_0}{H}\frac{H}{\delta}\right) + \frac{1}{2}\right), \qquad (35)$$

where δ corresponds to a length characteristic of the transition region ($\delta/H = 0.1$ in Fig. (**6**)), S_p is the value of the source term in the homogeneous porous region and the source term is considered as null in the free fluid region. The source surface-excess quantity is given by:

$$S_1^{ex} = \int_{-\infty}^{y_M}(S_1(y)-S_p)dy + \int_{y_M}^{+\infty}(S_1(y)-0)dy. \tag{36}$$

Its value does depend on the exact location of the interface inside the transition region as expected and illustrated in Fig. (**6**)(a) where two different positions of the interface have been plotted.
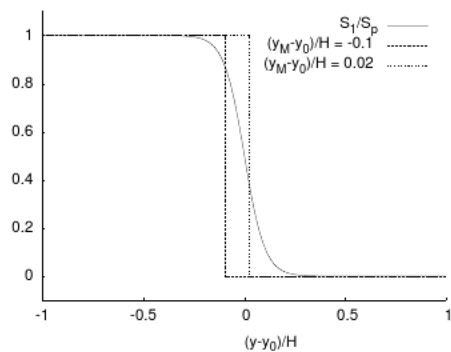
(a) Different asymptotic values: $\Psi^+ \neq \Psi^-$
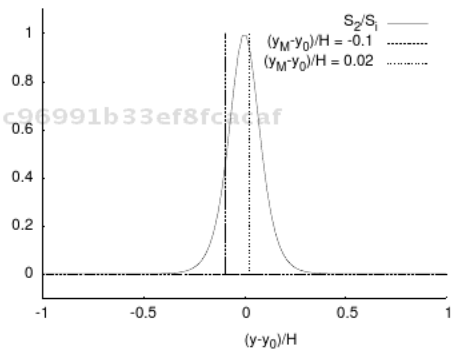
(b) Equal asymptotic values: $\Psi^+ = \Psi^-$

Fig. (**6**): Source terms used for the illustrative examples. Two different interface locations are represented inside the interfacial transition region.

Given the definition (32), the center of gravity y_{S_1} of the profile of S_1 is $y_{S_1} = y_0$ and the value of the

surface excess quantity is simply given by (33):

$$S_1^{ex} = (y_{S_1} - y_M)S_p. \tag{37}$$

Thus, for $(y_M - y_0)/H = -0.1$ its value is positive $S_1^{ex} = 0.1S_pH$ and for $(y_M - y_0)/H = 0.02$ its value is negative $S_1^{ex} = -0.02S_pH$. However, this dependence of the excess quantity on the location of the interface compensates the fact that the source term is different in the two homogeneous regions, equal to S_p in the porous region, and null in the free fluid region. However, one can verify, that the same overall source term is considered, whatever the location of the interface.

To illustrate this point, we present in Fig. (**7**)

- the solution obtained at the mesoscopic scale by solving equation (26)

- the solutions obtained at the macroscopic scale by solving equations (27) and (28) using the boundary conditions (29) and (30) for three different positions of the interface. The values of the excess quantities are presented in Table 1.

Figure (**7**) shows that the macroscopic problem is indeed equivalent to the mesoscopic one, whatever the position of the interface in the interfacial region. Indeed, outside of the transition region, the solutions are the same. Inside the transition region, since for the macroscopic problem, the source term is constant and not variable, the exact mesoscopic solution is not captured by the model. However, the overall transfers are captured, whatever the location of the interface, thanks to the appropriate jump parameters. This example illustrates the fact that jump parameters are not intrinsic quantities when $\Psi_- \neq \Psi^+$, since their value does depend on the location of the interface (Table 1).

For any properties whose asymptotic values are different, one *should* expect a dependence of the related jump parameters on the location of the interface.

Table 1: Value of the excess quantities for different position of the interface.

y_M/H	$(S_1)^{ex}$	$(q_1)^{ex}$	$(S_2)^{ex}$	$(q_2)^{ex}$
-0.1	- 0.1	-0.00891291	0.2	-0.02
0	0	- 0.00411291	0.2	0.
0.1	0.1	-0.00931291	0.2	0.02

3.2.2. Another Simple Source Term

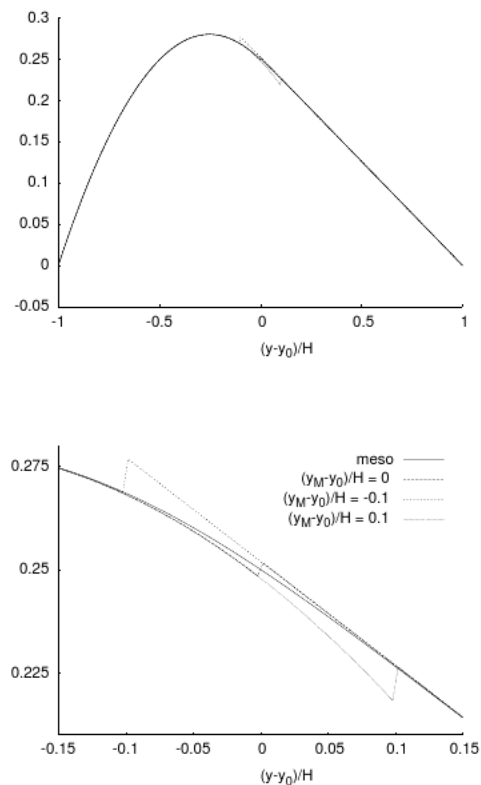Now, we consider another source term which is such that its values are the same in the two homogeneous

point in Fig. (**8**) where the mesoscopic and macroscopic solutions obtained with the source term (38) are presented. The values of the excess quantities are presented in Table 1. The surface-excess quantity S_2^{ex} does not depend on the interface location, since its two asymptotic values are the same. However, for q_2^{ex}, since its two asymptotic values are different, its value does depend on the interface location. As we can see in Fig. (**8**), the macroscopic solutions are indeed equivalent to the mesoscopic one, whatever the location of the interface inside the transition region.
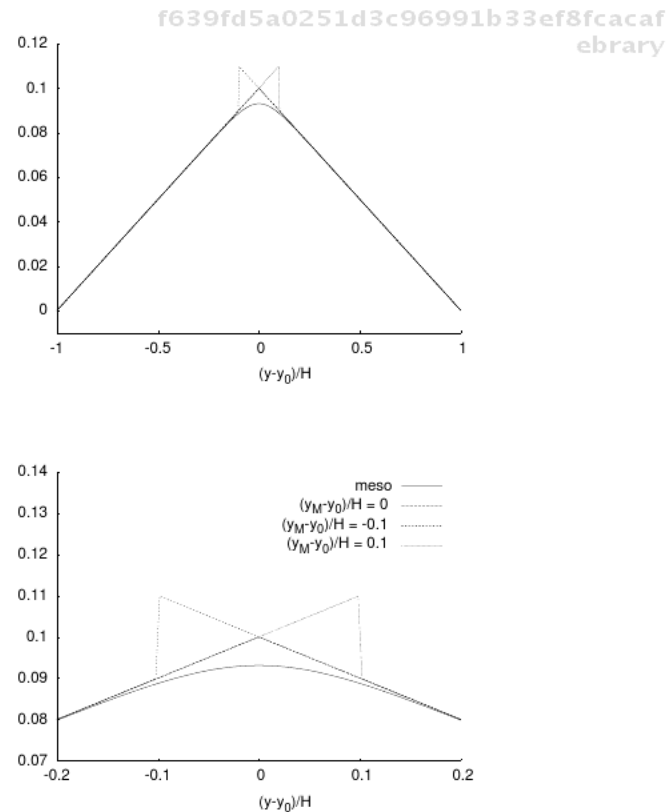
Fig. (**7**): Source term S_1: Comparison of the mesoscopic and macroscopic solutions for different positions of the interface. Zoom on the interfacial region

regions, as illustrated in Fig. (**6**)(b):

$$S_2(y) = S_i \left(1 - \left(\tanh \left(\frac{y - y_0}{H} \frac{H}{\delta} \right) \right)^2 \right). \quad (38)$$

Here, S_i is the amplitude of the source term variations in the transition region, the source term being considered as null in the homogeneous free fluid and porous regions. The source surface-excess quantity is given by:

$$S_2^{ex} = \int_{-\infty}^{+\infty} S_2(y). \quad (39)$$

Its value does not depend on the exact location of the interface inside the transition region as expected and illustrated in Fig. (**6**)(b) where two different positions of the interface have been plotted. The fact that the jump coefficient do not depend on the interface location is coherent with the fact that the source terms are the same in the two homogeneous regions. As with the previous example, we illustrate this

Fig. (**8**): Source term S_2: Comparison of the mesoscopic and macroscopic solutions for different positions of the interface. Zoom on the interfacial region

3.3. A Second Closure Problem

The surface-excess theory is a very powerful method, which allows to traduce a continuous model into a discontinuous one with boundary conditions such that the overall transfers are conserved in the up-scaling process. In particular, using this method,

one can show that the jump parameters are in fact surface-excess quantities. Thus, one can apprehend the dependence between the jump parameter's value and the location of the interface inside the transition region, as illustrated in the two previous examples. The equality (or not) of the two asymptotic values of the property involved in the surface-excess quantity is crucial in this dependence. Furthermore, the generic approach of the surface-excess theory is a quite general method that can be used to study many different transport equations.

Nevertheless, the generic approach of the surface-excess theory is not always sufficient. In the two previous simplified examples, the obtained boundary conditions were closed. However, this is not the case for the general three-dimensional case presented in section 3.1. The boundary conditions (21) and (25) are not closed at the macroscopic scale, since they involve mesoscopic unknowns in the surface-excess quantities. The two jump conditions need to be closed to relate the surface-excess quantities to averaged unknowns of the homogeneous regions.

To perform this second closure, different methods are used in the literature. To present them, we consider the diffusive-reactive mass transfer process in the one-dimensional and stationary case. From the surface-excess theory, we know that the *exact* jump conditions are:

$$[\tilde{c}_l - \tilde{c}_p]_{y_M} = -\left(\frac{q}{\phi D}\right)^{ex} \qquad (40)$$

$$\left[-D_l \frac{\tilde{c}_l}{dy} + \phi_p D_p \frac{\tilde{c}_p}{dy}\right]_{y_M} = \left(k\langle c\rangle^f\right)^{ex}. \qquad (41)$$

To close these relations, one can *postulate* the continuity of the concentration and a linear closure for the mass flux jump:

$$[\tilde{c}_l - \tilde{c}_p]_{y_M} = 0 \qquad (42)$$

$$\left[-D_l \frac{\tilde{c}_l}{dy} + \phi_p D_p \frac{\tilde{c}_p}{dy}\right]_{y_M} = \beta \tilde{c}_l, \qquad (43)$$

where β is a jump parameter. This type of approach has been followed by Ochoa-Tapia and Whitaker [19] for the study of the momentum transfer at the interface. However, by doing this, one losses the information related to the potential impact of the interface location. And it turns out that this impact is important for momentum transfer as observed in various contributions (Saffman [23], Larson & Higdon [16], Sahraoui & Kaviany [25], Breugem *et al.* [3] and Duman & Shavit [10]).

More recently, another approach has been proposed (Wood *et al.* [32]; Valdés-Parada *et al.* [28, 29, 30]), to *derive* these type of closure relations. However, at the end, the information related to the potential impact of the interface location is not very clear.

We present here another approach, namely the matched asymptotic expansion method, which allows to *derive* closure relations for the right-hand side of the jump conditions (40) and (41) without loosing information about the importance of the interface location. This approach has been applied with success in (Chandesris and Jamet [5, 6] to study the momentum transfer at a fluid-porous interface and thus to justify mathematically the observed dependence of the momentum jump parameter β of relation (2) to the interface location.

3.4. Matched Asymptotic Expansion Method

The idea of this method (see e.g. Dyke [11], Zwillinger [34]) is to solve analytically, using an asymptotic expansion in ε, the equations governing the problem at the mesoscopic scale:

$$0 = \frac{d}{dy}\left(\phi(y)D(y)\frac{dc}{dy}\right) + k(y)\,c. \qquad (44)$$

This asymptotic expansion is feasible because a small parameter, $\varepsilon = \delta/H$, is present in the mesoscopic equation (44) through the porosity, diffusivity and reaction rate profiles. As ε tends to zero, the transition region tends to a discontinuous surface. Thus, the result obtained using the asymptotic expansion is both an approximated solution at a given order of the mesoscopic problem and the solution of a macroscopic problem with a discontinuous interface for which the boundary conditions can be made explicit. Thus, this method allows to derive analytically, and at a given order, the boundary conditions of the macroscopic problem such that the macroscopic problem is indeed equivalent to the mesoscopic one.

The technical steps of the method and in particular the origin of the matching conditions are given for completeness concern.

The resolution domain is dividing in different sub-regions: an *outer region*, where the variables of the system are slowly varying, and an *inner region*, where these variables are rapidly varying. In our study, the transition zone is the inner region where the variables such as the porosity, the diffusivity, the reaction rate and the concentration are rapidly

varying, while each homogeneous region (porous medium and free fluid) is an outer region.

A change of variable is made in the inner region, since variations of order one are expected to take place in this thin region and a new space variable is introduced:

$$\check{y} = \frac{y - y_M}{\varepsilon} \qquad (45)$$

Let f be any physical variable. Then, $\check{f}$ is introduced in the inner region:

$$\check{f}(\check{y}) = f(y). \qquad (46)$$

$\check{f}(\check{y})$ varies more slowly than $f(y)$ in the inner region. Hereafter, the notation f will designate any variable in the outer regions, while $\check{f}$ will designate this variable in the inner region.

The differential equations are solved separately in each region, using an asymptotic expansion in ε. For example, at first order, the solutions are sought for in the form:

$$f(y, \varepsilon) = f^{(0)}(y) + \varepsilon f^{(1)}(y) + \mathcal{O}(\varepsilon^2) \quad (47)$$
$$\check{f}(\check{y}, \varepsilon) = \check{f}^{(0)}(\check{y}) + \varepsilon \check{f}^{(1)}(\check{y}^+) + \mathcal{O}(\varepsilon^2).(48)$$

However, in order to solve completely the differential equations in each region, boundary conditions are needed. The missing boundary conditions are obtained by matching the solutions of the different regions using the following matching principles [34]:

$$\lim_{y \to y_M^+} f(y, \varepsilon) = \lim_{\check{y} \to +\infty} \check{f}(\check{y}, \varepsilon) \hat{=} f_i^+ \qquad (49)$$

$$\lim_{y \to y_M^-} f(y, \varepsilon) = \lim_{\check{y} \to -\infty} \check{f}(\check{y}, \varepsilon) \hat{=} f_i^-. \qquad (50)$$

These relations mean that, for the study of the outer regions, the interface is viewed as a surface of discontinuity located in y_M^+ (respectively y_M^-), and for the study of the inner region, the outer regions are supposed to be reached asymptotically in $+\infty$ and $-\infty$. f_i^+ (respectively f_i^-) is the value of f at the interface "side $^+$" (respectively "side $^-$", and is the same in the inner and the outer studies.

Relations (49) and (50) are then made explicit. Using an asymptotic expansion of $f^{(0)}(y)$ as $y \to y_M^+$ (respectively $y \to y_M^-$), equation (47) can be rewritten at first order:

$$f(y, \varepsilon) = \lim_{y \to y_M^{\pm}} f^{(0)}(y)$$
$$+\varepsilon \left(\check{y} \lim_{y \to y_M^{\pm}} \frac{df^{(0)}}{dy} + \lim_{y \to y_M^{\pm}} f^{(1)}(y) \right) + \mathcal{O}(\varepsilon^2). \qquad (51)$$

Using equations (48), (49), (50) and (51), the following matching conditions are obtained at first order:

$$\lim_{\check{y} \to \pm\infty} \check{f}^{(0)} = \lim_{y \to y_M^{\pm}} f^{(0)}, \qquad (52)$$

$$\lim_{\check{y} \to \pm\infty} \check{f}^{(1)} = \lim_{y \to y_M^{\pm}} f^{(1)} + \check{y} \lim_{y \to y_M^{\pm}} \frac{df^{(0)}}{dy}. \qquad (53)$$

Following this approach, matching conditions can be derived at higher order and for the derivatives of f. In this study, the following matching conditions will also be used:

$$\lim_{\check{y} \to \pm\infty} \frac{d\check{f}^{(0)}}{d\check{y}} = 0, \qquad (54)$$

$$\lim_{\check{y} \to \pm\infty} \frac{d\check{f}^{(1)}}{d\check{y}} = \lim_{y \to y_M^{\pm}} \frac{df^{(0)}}{dy}, \qquad (55)$$

$$\lim_{\check{y} \to \pm\infty} \frac{d\check{f}^{(2)}}{d\check{y}} = \lim_{y \to y_M^{\pm}} \frac{df^{(1)}}{dy} + \check{y} \lim_{y \to y_M^{\pm}} \frac{d^2 f^{(0)}}{dy^2}. \qquad (56)$$

Using these relations to match the solutions in the different regions, an approximate solution of the equations is obtained in the whole domain. Further explanations about this method can be found in Dyke [11], Zwillinger [34] and Zeytounian [11].

3.4.1. Outer Region

To make an asymptotic expansion in ε of equation (44), we need to specify the variations of the porosity, the diffusivity and the reaction rate in the outer region. At this point, we just assume that they are constant in each homogeneous region at least to second order. This means, for the porosity for example:

$$\phi = \phi^{(0)} + \mathcal{O}(\varepsilon^2) = \begin{cases} \phi_p + \mathcal{O}(\varepsilon^2), & y < y_M \\ 1 + \mathcal{O}(\varepsilon^2), & y > y_M \end{cases}. \qquad (57)$$

Such variations can be obtained by considering profiles as those presented in Fig. (**6**).

In the outer region, the solution is sought for in the form:

$$c(y, \varepsilon) = c^{(0)}(y) + \varepsilon c^{(1)}(y) + \mathcal{O}(\varepsilon^2). \qquad (58)$$

Thus, at order i, equation (44) reduces to:

$$0 = \frac{d}{dy} \left(\phi^{(0)} D^{(0)} \frac{dc^{(i)}}{dy} \right) + k^{(0)} c^{(i)}, \quad i = 0, 1. \qquad (59)$$

3.4.2. Inner Region

In order to study the inner problem, the space variable (45) is used. Using this variable, equation (44) becomes:

$$0 = \frac{1}{\varepsilon^2}\frac{d}{d\check{y}}\left(\check{\phi}(\check{y})\check{D}(\check{y})\frac{d\check{c}}{d\check{y}}\right) + \check{k}(\check{y})\,\check{c}. \qquad (60)$$

To solve this equation, we need to specify the functional dependence of the porosity, the diffusivity and the reaction rate in the transition zone. It is assumed that these functions are varying as y/δ. It only implies that they are rapidly varying in the transition zone, as expected. As a consequence, $\check{\phi}$ and $\check{D}$ and $\check{k}$ do not depend on ε, i.e. for the porosity for example $\check{\phi} = \check{\phi}^{(0)}$ without approximation.

In the inner region, the solution is sought for in the form:

$$\check{c}(\check{y},\varepsilon) = \check{c}^{(0)}(\check{y}) + \varepsilon\check{c}^{(1)}(\check{y}^+) + \mathcal{O}(\varepsilon^2). \qquad (61)$$

The asymptotic expansion in ε of equation (60) reads:

Order 0: $\qquad 0 = \frac{d}{d\check{y}}\left(\check{\phi}\check{D}\frac{d\check{c}^{(0)}}{d\check{y}}\right), \qquad (62)$

Order 1: $\qquad 0 = \frac{d}{d\check{y}}\left(\check{\phi}\check{D}\frac{d\check{c}^{(1)}}{d\check{y}}\right), \qquad (63)$

Order 2: $\qquad \frac{d}{d\check{y}}\left(\check{\phi}\check{D}\frac{d\check{c}^{(2)}}{d\check{y}}\right) = -\check{k}\,\check{c}^{(0)}. \qquad (64)$

3.4.3. Zeroth Order Solution

Solving equation (62) leads to:

$$\frac{d\check{c}^{(0)}}{d\check{y}} = \frac{k_1}{\check{\phi}\check{D}}, \qquad (65)$$

where k_1 is a constant of integration. Using the matching condition (54) and the fact that $\check{\phi}$ and $\check{D}$ do not cancel at $\pm\infty$, it comes that $k_1 = 0$. This implies that $\check{c}^{(0)}$ is a constant. Using the matching condition (52), one has:

$$\check{c}^{(0)} = c^{(0)}\big|_{y_M^+} = c^{(0)}\big|_{y_M^-}. \qquad (66)$$

At zeroth order, the concentration is continuous at the fluid-porous interface.
To obtain a condition on the mass flux, we solve equation (63). This yields

$$\check{\phi}\check{D}\frac{d\check{c}^{(1)}}{d\check{y}} = k_2, \qquad (67)$$

where k_2 is a constant of integration. Using the matching conditions (55) and (52), one has:

$$\lim_{\check{y}\to+\infty}\check{\phi}\check{D}\frac{d\check{c}^{(1)}}{d\check{y}} = D_l\frac{dc^{(0)}}{dy}\Big|_{y_M^+} = k_2, \qquad (68)$$

$$\lim_{\check{y}\to-\infty}\check{\phi}\check{D}\frac{d\check{c}^{(1)}}{d\check{y}} = \phi_p D_p\frac{dc^{(0)}}{dy}\Big|_{y_M^-} = k_2, \qquad (69)$$

which implies:

$$-D_l\frac{dc^{(0)}}{dy}\Big|_{y_M^+} + \phi_p D_p\frac{dc^{(0)}}{dy}\Big|_{y_M^-} = 0. \qquad (70)$$

At zeroth order, the mass flux is continuous at the fluid-porous interface and we note:

$$\begin{aligned} q^{(0)}\big|_{y_M} &= -D_l\frac{dc^{(0)}}{dy}\Big|_{y_M^+} = -\phi_p D_p\frac{dc^{(0)}}{dy}\Big|_{y_M^-} \\ &= -\check{\phi}\check{D}\frac{d\check{c}^{(1)}}{d\check{y}}. \end{aligned} \qquad (71)$$

The solution of the mesoscopic problem (44) at zeroth order is the quantity $c^{(0)}$ which verifies the governing equation (59) in each homogeneous region and the boundary conditions (66) and (71). Thus, using the continuity of both the concentration and the mass flux gives an approximate solution at zeroth order of the mesoscopic problem (44).

3.4.4. First Order Solution

To find the boundary condition at first order, we first rearrange equation (67) in the following forms using the definition of the zeroth order mass flux:

$$\frac{d}{d\check{y}}\left(\check{c}^{(1)} - \check{y}\frac{dc^{(0)}}{dy}\Big|_{y_M^+}\right) = -q^{(0)}\big|_{y_M}\left(\frac{1}{\check{\phi}\check{D}} - \frac{1}{D_l}\right), \qquad (72)$$

$$\frac{d}{d\check{y}}\left(\check{c}^{(1)} - \check{y}\frac{dc^{(0)}}{dy}\Big|_{y_M^-}\right)$$
$$= -q^{(0)}\big|_{y_M}\left(\frac{1}{\check{\phi}\check{D}} - \frac{1}{\phi_p D_p}\right). \qquad (73)$$

Equation (73) is integrated from $\check{y} = -\infty$ to $\check{y} = 0$. Using the matching condition (53), we have:

$$\lim_{\check{y}\to-\infty}\left(\check{c}^{(1)} - \check{y}\frac{dc^{(0)}}{dy}\right) = c^{(1)}\big|_{y_M^-}. \qquad (74)$$

Thus, one gets

$$\check{c}^{(1)}(0) - c^{(1)}\big|_{y_M^-} = -q^{(0)}\big|_{y_M}$$
$$\int_{\check{y}=-\infty}^{\check{y}=0}\left(\frac{1}{\check{\phi}\check{D}} - \frac{1}{\phi_p D_p}\right)d\check{y}. \qquad (75)$$

In the same way, equation (72) is integrated from $\breve{y} = 0$ to $\breve{y} = +\infty$. Adding the two results, it yields

$$c^{(1)}\big|_{y_M^+} - c^{(1)}\big|_{y_M^-} = -q^{(0)}\big|_{y_M}$$
$$\left[\int_{\breve{y}=-\infty}^{\breve{y}=0} \left(\frac{1}{\breve{\phi}\breve{D}} - \frac{1}{\phi_p D_p} \right) d\breve{y} \right. \tag{76}$$
$$\left. + \int_{\breve{y}=0}^{\breve{y}=+\infty} \left(\frac{1}{\breve{\phi}\breve{D}} - \frac{1}{D_l} \right) d\breve{y} \right].$$

And after a change of variable, one obtains

$$\varepsilon \left(c^{(1)}\big|_{y_M^+} - c^{(1)}\big|_{y_M^-} \right) = -q^{(0)}\big|_{y_M} \left(\frac{1}{\phi D} \right)^{ex}, \quad (77)$$

where the excess-quantity is defined by equation (31).

To obtain a condition on the mass flux, we study equation (64) and rearrange it in the following form, using first the outer equation at zeroth order in the free fluid region (59):

$$\frac{d}{d\breve{y}} \left(\breve{\phi}\breve{D} \frac{d\breve{c}^{(2)}}{d\breve{y}} - \breve{y} \left(D_l \frac{d^2 c^{(0)}}{d^2 y}\Big|_{y_M^+} \right) \right) = -\breve{k}\, \breve{c}^{(0)}, \tag{78}$$

then, the outer equation at zeroth order in the porous region

$$\frac{d}{d\breve{y}} \left(\breve{\phi}\breve{D} \frac{d\breve{c}^{(2)}}{d\breve{y}} - \breve{y} \left(\phi_p D_p \frac{d^2 c^{(0)}}{d^2 y}\Big|_{y_M^-} \right) \right) =$$
$$- \left(\breve{k}\, \breve{c}^{(0)} - k_p\, c^{(0)}\big|_{y_M^-} \right). \tag{79}$$

Equation (78) is integrated from $\breve{y} = -\infty$ to $\breve{y} = 0$. Using the matching condition (56), we have:

$$\lim_{\breve{y} \to -\infty} \left(\breve{\phi}\breve{D} \frac{d\breve{c}^{(2)}}{d\breve{y}} - \breve{y} \left(\phi_p D_p \frac{d^2 c^{(0)}}{d^2 y} \right) \right) =$$
$$\phi_p D_p \frac{dc^{(1)}}{dy}\Big|_{y_M^-}. \tag{80}$$

Thus, since the inner concentration is constant at zeroth order (66) one gets

$$\left(\breve{\phi}\breve{D} \frac{d\breve{c}^{(2)}}{d\breve{y}} \right)(0) - \phi_p D_p \frac{dc^{(1)}}{dy}\Big|_{y_M^-} =$$
$$- c^{(0)}\big|_{y_M} \int_{\breve{y}=-\infty}^{\breve{y}=0} \left(\breve{k} - k_p \right) d\breve{y}. \tag{81}$$

In the same way, equation (79) is integrated from $\breve{y} = 0$ to $\breve{y} = +\infty$. Adding the two results, and after a change of variables, we obtain

$$\varepsilon \left(-D_l \frac{dc^{(1)}}{dy}\Big|_{y_M^+} + \phi_p D_p \frac{dc^{(1)}}{dy}\Big|_{y_M^-} \right) = c^{(0)}\big|_{y_M} (k)^{ex}. \tag{82}$$

The solution of the mesoscopic problem (44) at first order is the quantity $\tilde{c} = c^{(0)} + \varepsilon c^{(1)}$ which verifies the governing equation (59) in each homogeneous region and the following boundary conditions at the fluid-porous interface:

$$\tilde{c}\big|_{y_M^+} - \tilde{c}\big|_{y_M^-} = -q^{(0)}\big|_{y_M} \left(\frac{1}{\phi D} \right)^{ex}, \quad (83)$$

$$-D_l \frac{d\tilde{c}}{dy}\Big|_{y_M^+} + \phi_p D_p \frac{d\tilde{c}}{dy}\Big|_{y_M^-} = c^{(0)}\big|_{y_M} (k)^{ex}. \quad (84)$$

We obtain a jump both on the concentration and on the mass flux. Compared to equations (40) and (41), these boundary conditions are closed since they involved only macroscopic variables or surface-excess quantities of properties that are known. Indeed, since the properties in the homogeneous regions are constant and different, the excess quantities can be rewritten using equation (33) and this gives

$$\tilde{c}\big|_{y_M^+} - \tilde{c}\big|_{y_M^-} = -q^{(0)}\big|_{y_M} \left(\frac{1}{D_l} - \frac{1}{\phi_p D_p} \right) (y_M - y_{1/\phi D}), \tag{85}$$

$$-D_l \frac{d\tilde{c}}{dy}\Big|_{y_M^+} + \phi_p D_p \frac{d\tilde{c}}{dy}\Big|_{y_M^-} = c^{(0)}\big|_{y_M} (-k_p)(y_M - y_k). \tag{86}$$

Thus, the jump relations at order 1 depend on intrinsic interfacial properties: $y_{1/\phi D}$ and y_k, the *center of gravity* of respectively $1/(\phi D)$ and k; on the location of the interface y_M and on the properties of the homogeneous media: ϕ_p, D_p, D_l, k_p. The information about the influence of the interface location is kept *via* the two surface-excess quantities k^{ex} and $(1/\phi D)^{ex}$. Indeed, if we set $\beta = k^{ex}$, we see that the value of the jump parameter depends on the interface location.

It should be pointed out that, regarding the resolution of this macroscopic problem, the first order solution is obtained in two steps. First, it is necessary to solve the macroscopic model at zeroth order to obtain the value of $q^{(0)}\big|_{y_M}$ and $c^{(0)}\big|_{y_M}$. Then, the macroscopic model at order one can be solved.

3.5. A First Overlook

In this section, we have shown how a continuous model of the interface can be traduced into a discontinuous one with its associated boundary conditions. In particular, we have shown that these boundary conditions are related to surface-excess quantities whose values can depend on the interface location. This is particularly the case when studying fluid-porous problem, for which the asymptotic values of the governing properties are different in the

two homogeneous regions. Furthermore, we have presented two different tools to study this continuous/discontinuous up-scaling process.

4. DISCUSSION

The main idea behind our two-step modeling approach of the interface, is to dissociate the modeling difficulty associated to the physical modeling specific of the transfers in the interfacial fluid/porous region from the modeling difficulty of using a discontinuous description to model these specific interfacial transfers. Using this approach, we have shown that the jump parameters that appear in the jump conditions can be interpreted as surface-excess quantities and thus can depend on the interface location. The jump parameters are not necessarily *intrinsic* interfacial parameters.

4.1. Intrinsic versus Non-Intrinsic Nature of the Jump Coefficients

In the present two-step modeling approach, the transfers specific of the interfacial transition region are taken into account, at the mesoscopic scale, through variations of the medium properties (permeability, porosity, effective conductivity or diffusivity, ...). Now, regarding the variations of these properties, different situations can be faced, as illustrated in Fig. (**9**).

The property involved in the jump parameter via its excess-quantity can be such that its two-asymptotic values are equal, as illustrated in Fig. (**9**)(a). In this case, the excess-quantity does not depend on the interface location and the jump parameter is indeed an intrinsic interfacial parameter. We have never faced such situations while studying fluid-porous transfers, but this situation is typical of the van de Waals theory of capillarity in which the surface tension is interpreted as a surface-excess energy [22].

For fluid-porous transfers, the property involved in the jump parameter *via* its excess-quantity is usually such that its two-asymptotic values are different (porosity, permeability, effective conductivity or diffusivity, ...). In this case the excess-quantity value depends on the interface location. However, it can be shown that the excess-quantity can be divided in two parts: an intrinsic part that is independent of the interface location and a variable part (see Jamet & Chandesris [15] for more details).

If the variable part is small compared to the intrinsic part, as illustrated in Fig. (**9**)(b), then, whatever the interface position y_M within the transition zone, the value of the surface-excess quantity ψ^{ex} is almost

equal to its intrinsic part. In this case, no significant variation of the solution in the homogeneous regions is observed as the interface position y_M varies. In this case, the jump parameter appears as an intrinsic interfacial parameter and the precise location of the interface inside the transition region is not crucial. This type of situation is encountered when studying turbulent flows perpendicular to a fluid/porous interface. The pressure drop at the interface is modeled using a singular pressure drop coefficient. Even though the two-asymptotic values of the friction coefficient are different, no dependence of the singular pressure drop coefficient on the precise location of the interface is reported. This is because the variable part of the involved excess-quantity is negligible compared to its intrinsic part.

When the variable part of the surface-excess quantity is of the same order of magnitude as its intrinsic part (see Fig. (**9**)(c)), as the interface position y_M varies within the interfacial transition zone, the solution of the problem in the homogeneous regions may vary significantly. In this case, it is important to define the position of the interface and the corresponding surface-excess quantity precisely to recover the correct solution. In this case, the jump parameter is not an intrinsic property. The intrinsic property that characterizes without ambiguity the interfacial region is the center of gravity y_Ψ of the quantity involved in the surface-excess.

4.2. Apparent Interface Location

In this last case, when the jump parameter is not an intrinsic property, the use of a jump condition is not as necessary as originally thought. Indeed, in this case, the jump parameter's value cancels for $y_M = y_\Psi$ and the continuity condition can thus be used at this particular position of the interface. This particular position of the interface for which boundary conditions of continuity are sufficient, is named the *apparent interface* by Duman & Shavit [10].

This alternative approach is very interesting to avoid the numerical implementation of the jump conditions and the two-step numerical resolution when the boundary conditions involve zeroth and first order solutions as in (83) and (84).

However, the existence of an apparent interface is not always guaranteed, especially (i) when two jump conditions are involved as in the mass transfer process presented in section 3.1, (ii) when more than one excess-quantity is involved in the jump condition or (iii) when the intrinsic part is dominant in the jump parameter. Nevertheless, the alternative
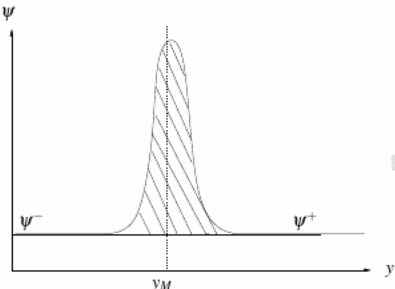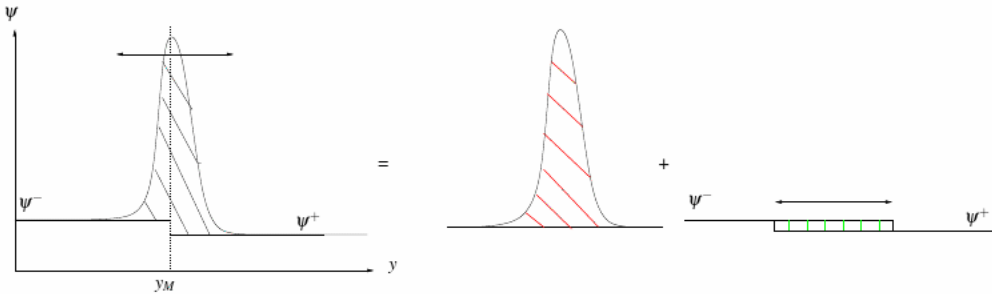
(a) $\Psi^+ = \Psi^-$

(b) $\Psi^+ \neq \Psi^-$: A big intrinsic part and a small variable part
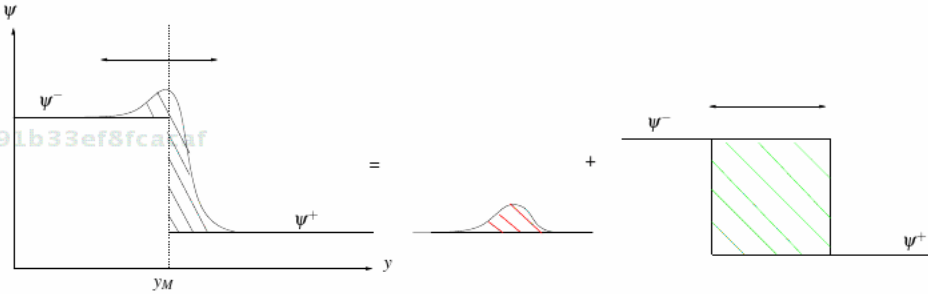
(c) $\Psi^+ \neq \Psi^-$: A small intrinsic part and a big variable part

Fig. (**9**): Intrinsic versus non-intrinsic nature of the coefficient

approach of the apparent interface seems very interesting for the study of practical applications and the questions of its existence and its location can be investigated using the two-step approach as done for example in D'Hueppe *et al.* [9] for a 2D convective heat transfer problem.

CONCLUSIONS

In this chapter, we analyze the jump conditions that must be imposed at a fluid/porous interface in order to account for the transfers that occur in the interfacial region. This general analysis is based on three different descriptions of the interface and two up-scaling steps.

The first one allows to obtain a continuous description of the problem. The transfers in the interfacial region are modeled *via* effective properties (porosity, permeability, diffusivity, ...) that vary in the interfacial transition regions. These effective properties are usually determined by matching the volume averaged fields obtained by volume averaging microscopic simulations or experimental data with the solution of the model in the interfacial region. The physics of the transfers and their potential specificities in the interfacial region is thus characterized at this continuous scale.

Then, a second up-scaling step is performed. Two different methods are presented here: the generic approach of the surface-excess theory and the matched asymptotic expansion method. In both methods, the physical features that are not (or not correctly) accounted for by the macroscopic model, compared to the mesoscopic one, in the interfacial region, are assigned to the interface through jump conditions that involve surface-excess quantities. Depending on the studied property, its associated excess-quantity can depend on the interface location. This dependence compensates the fact that the macroscopic models are different in the two homogeneous regions and that changing the interface location, modifies the zone of influence of a given macroscopic model.

The generic approach of the surface-excess theory is very general and can be used to study many different transport equations. However, the boundary conditions obtained with this method involve surface-excess quantities that are generally not closed. To close these excess quantities, a common approach was to *postulate* their form: continuity, linear closure, ... We present here another approach, namely the matched asymptotic expansion method, which allows to formally *derive* closure relations for these unclosed surface-excess quantities.

Given these results, it is possible to analyze the physical nature of the jump coefficients and to determine whether they are intrinsic parameters or not. In general, for fluid-porous transfers, the jump coefficients do depend on the interface location and are not intrinsic. However, if their variable part is negligible compared to their intrinsic part, they can appear as intrinsic parameters.

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