# ANALYSIS OF TURBULENT MASS TRANSPORT IN SATURATED POROUS MEDIA

**Maximilian S. Mesquita**
**Marcelo J.S. De-Lemos***
Departamento de Energia - IEME
Instituto Tecnológico de Aeronáutica - ITA
12228-900 - São José dos Campos - SP - Brazil
*Corresponding Author. E-mail: delemos@mec.ita.br

***Abstract.*** *This paper presents derivations of mass transport equations for turbulent flow in permeable structures. Equations are developed following two distinct procedures. The first method considers time averaging of the local instantaneous mass transport equation before the volume average operator is applied. The second methodology employs both averaging operators but in a reverse order. This work is intended to demonstrate that both approaches lead to equivalent equations when one takes into account both time fluctuations and spatial deviations of velocity and mass fraction. A modeled form for the final transport equation is presented where turbulent transfer is based on a macroscopic version of the k-ε model.*

***Keywords*** *.Turbulence Model, Porous Media, Mass Transfer*

## 1. Introduction

Modeling of macroscopic transport for incompressible flows in rigid porous media has been based on the volume-average methodology for either heat [1] or mass transfer [2-5]. If time fluctuations of the flow properties are considered, in addition to spatial deviations, there are two possible methodologies to follow in order to obtain macroscopic equations: *a*) application of time-average operator followed by volume-averaging [6-9], or *b*) use of volume-averaging before time-averaging is applied [10-13]. This work is intended to show that both sets of macroscopic mass transport equations are equivalent when examined under the recently established *double decomposition* concept [14-17]. This methodology, initially developed for the flow variables, has been extended to heat transfer in porous media where both time fluctuations and spatial deviations were considered for velocity, temperature and Mass [18, 20]. A general classification of all proposed models for turbulent flow and heat transfer in porous media has been recently published [19]. Here, mass transport is considered and a methodology for calculating the dispersion coefficients is described.

## 2. Mathematical Model

### 2.1 Local Instantaneous Mass Transport Equations

The mass fraction distribution for the chemical species $\ell$ is governed by the following transport equation,

$$\frac{\partial \rho\, m_\ell}{\partial t} + \nabla \cdot (\, \rho\, \mathbf{u}\, m_\ell + \mathbf{J}_\ell\,) = \rho\, R_\ell \tag{1}$$

where $m_\ell$ is the mass fraction of component $\ell$, defined as $m_\ell = \dfrac{\rho_\ell}{\rho}$, $\rho_\ell$ is the mass density of species $\ell$ (mass of $\ell$ over total volume) and $\rho$ is the bulk density of the mixture ( $\rho = \sum_\ell \rho_\ell$ ). Also, $\mathbf{u}$ is the mass-averaged velocity of the mixture, $\mathbf{u} = \sum_\ell m_\ell \mathbf{u}_\ell$ , where $\mathbf{u}_\ell$ is the velocity of species $\ell$. Further, the mass diffusion flux $\mathbf{J}_\ell$ in (1) is due to the velocity slip of species $\ell$,

$$\mathbf{J}_\ell = \rho_\ell (\mathbf{u}_\ell - \mathbf{u}) = -\rho D_\ell\, \nabla m_\ell \tag{2}$$

where $D_\ell$ is the diffusion coefficient of species $\ell$ into the mixture. The second equality in equation (2) is known as Fick's Law. This constitutive equation is strictly valid for binary mixtures under the absence of any additional driving mechanisms for mass transfer [2]. The generation rate of species $\ell$ per unit of mixture mass is given in (1) by $R_\ell$.

As mentioned, there are, in principle, two ways that one can follow in order to treat turbulent flow in porous media. The first method applies a time average operator to the governing equation (1) before the volume average procedure is conducted. In the second approach, the order of application of the two average operators is reversed. Both techniques aim at derivation of a suitable macroscopic turbulent mass transport equation.

Volume averaging in a porous medium, described in detail in references [21-23], makes use of the concept of a Representative Elementary Volume (REV), see Figure 1, over which local equations are integrated. After integration, detailed information within the volume is lost and, instead, overall properties referring to a REV are considered. In a similar manner, statistical analysis of turbulent flow leads to time mean properties. Transport equations for statistical values are considered in lieu of instantaneous information on the flow.

Before undertaking the task of developing macroscopic equations, it is convenient to recall the definition of time average and volume average.

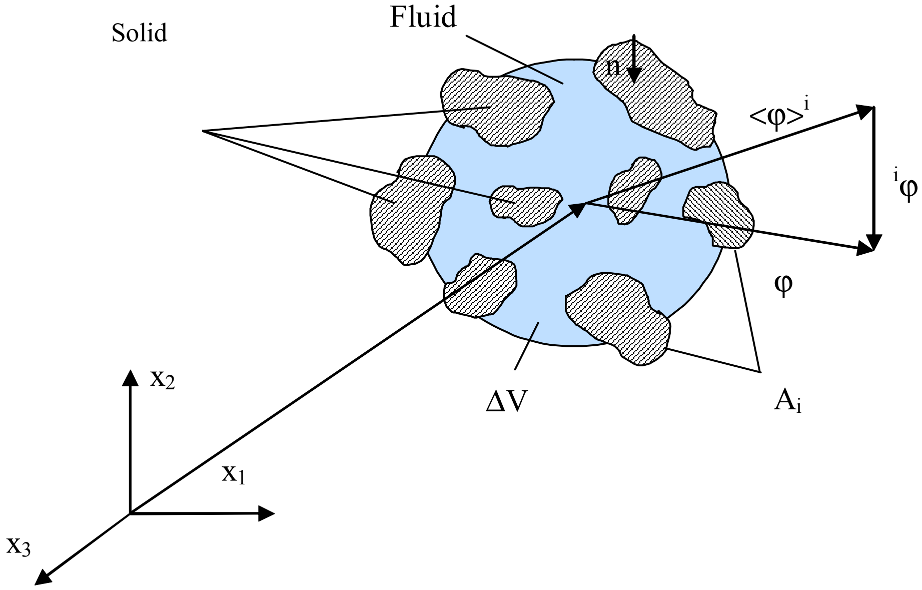


Figure 1 – REV, Intrisic average ;space and time fluctuations

### 2.2. Volume and Time Average Operators - Double Decomposition Concept

The volume average of $\varphi$ taken over a Representative Elementary Volume in a porous medium can be written as:

$$\langle\varphi\rangle^{v}=\frac{1}{\Delta V}\int_{\Delta V}\varphi\, dV \tag{3}$$

The value $\langle\varphi\rangle^{v}$ is defined for any point **x** surrounded by a Representative Elementary Volume, of size ΔV. This average is related to the *intrinsic* average for the fluid phase as:

$$\langle\varphi_f\rangle^{v}=\phi\langle\varphi_f\rangle^{i} \tag{4}$$

where $\phi=\Delta V_f/\Delta V$ is the medium porosity and $\Delta V_f$ is the volume occupied by the fluid in a REV. Furthermore, one can write:

$$\varphi=\langle\varphi\rangle^{i}+{}^{i}\varphi \tag{5}$$

with $\langle{}^{i}\varphi\rangle^{i}=0$. In equation (5), ${}^{i}\varphi$ is the *spatial deviation* of $\varphi$ with respect to the intrinsic average $\langle\varphi\rangle^{i}$.

Further, the local volume average theorem can be expressed as [21-23]:

$$\begin{aligned}
\langle\nabla\varphi\rangle^{v} &= \nabla(\phi\langle\varphi\rangle^{i})+\frac{1}{\Delta V}\int_{A_i}\mathbf{n}\varphi\, dS\\
\langle\nabla\cdot\boldsymbol{\varphi}\rangle^{v} &= \nabla\cdot(\phi\langle\boldsymbol{\varphi}\rangle^{i})+\frac{1}{\Delta V}\int_{A_i}\mathbf{n}\cdot\boldsymbol{\varphi}\, dS\\
\langle\frac{\partial\varphi}{\partial t}\rangle^{v} &= \frac{\partial}{\partial t}(\phi\langle\varphi\rangle^{i})-\frac{1}{\Delta V}\int_{A_i}\mathbf{n}\cdot(\mathbf{u}_i\varphi)\, dS
\end{aligned} \tag{6}$$

where **n** is the unit vector normal to the fluid-solid interface and $A_i$ is the fluid-solid interface area within the REV. It is important to emphasize that $A_i$ should not be confused with the surface area surrounding volume ΔV
Further, the time average of a general quantity $\varphi$ is defined as:

$$\overline{\varphi}=\frac{1}{\Delta t}\int_{t}^{t+\Delta t}\varphi\, dt \tag{7}$$

where the time interval $\Delta t$ is small compared to the fluctuations of the average value, $\overline{\varphi}$, but large enough to capture turbulent fluctuations of $\varphi$. Time decomposition can then be written as,

$$\varphi=\overline{\varphi}+\varphi' \tag{8}$$

with $\overline{\varphi'}=0$. Here, $\varphi'$ is the *time fluctuation* of $\varphi$ around its average $\overline{\varphi}$.

Pedras and de Lemos [14,15] showed that for a rigid, homogeneous porous medium saturated with an incompressible fluid, the following relationships apply:

$$\overline{\langle \varphi \rangle^i} = \langle \overline{\varphi} \rangle^i$$

$$\overline{\varphi} = \overline{{}^i\varphi} \tag{9}$$

$$\langle \varphi' \rangle^i = \langle \varphi \rangle^{i\,\prime}$$

Therefore, a general quantity $\varphi$ can be expressed by either,

$$\varphi = \overline{\langle \varphi \rangle^i} + \langle \varphi \rangle^{i\,\prime} + \overline{{}^i\varphi} + {}^i\varphi' \tag{10}$$

or

$$\varphi = \langle \overline{\varphi} \rangle^i + {}^i\overline{\varphi} + \langle \varphi' \rangle^i + {}^i\varphi' \tag{11}$$

Expressions (10) and (11) comprise the double decomposition concept where ${}^i\varphi'$ can be understood as either the *time fluctuation of the spatial deviation* or the *spatial deviation of the time fluctuation*. Also, $\langle {}^i\varphi' \rangle^i = \overline{{}^i\varphi'} = 0$ .

With the help of Figure 2, from 18, the concept of double decomposition proposed in 14 and 15 can be visualized. The Figure shows a three-dimensional diagram for a general vector variable $\varphi$ . For a scalar, all quantities shown would be drawn on a single line. Also, notice that points ***B***, ***C***, ***D*** and ***E*** fall in the same plane, with segments ***BC*** and ***BE*** parallel to ***ED*** and ***CD***, respectively. Line ***AEF*** represents standard time decomposition given by (8) whereas equation (5) is pictured by line ***ACF***. Further, (26) is given by line ***ABE*** and (18) by segment ***ABC***. The First Equality of equation (9) is represented by ***AB*** and other two equations in (9) by the equivalence between the parallel segments ***BE*** and ***CD*** and between ***BC*** and ***ED***. Triangles ***EDF*** and ***CDF*** are associated with the decomposition of the equations (9). Finally, equation (10) follow the sequence ***ABCDE*** and relationship (11) is represented by the path ***ABEDF***, both of them decomposing the same general variable $\varphi$ .

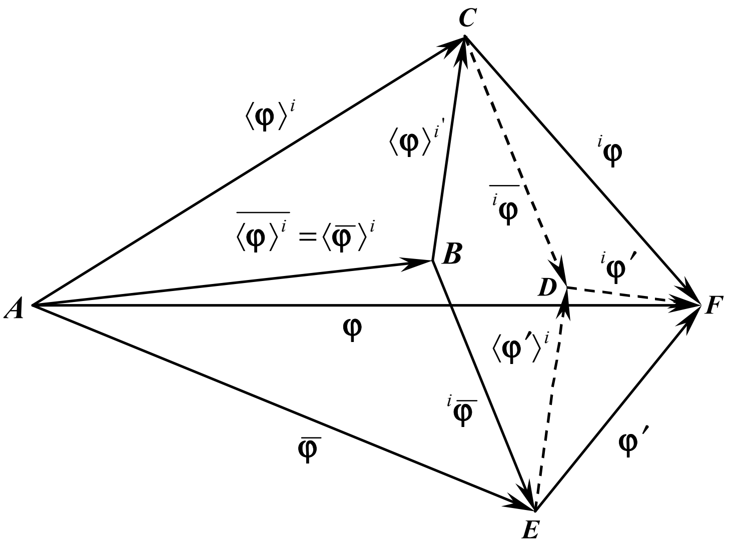


Figure 2 – General Three-dimensional vector diagram for a quantity $\varphi$

### 2.3. Macroscopic Time Averaged Mass Transport Equations

To apply the volume average to **(1)**, one has:

$$m_\ell = \langle m_\ell \rangle^i + {}^i m_\ell \tag{12}$$

$$\mathbf{u} = \langle \mathbf{u} \rangle^i + {}^i\mathbf{u} \tag{13}$$

Substituting (12) and (13) into (1), one obtains:

$$\frac{\partial (\langle m_\ell \rangle^i + {}^i m_\ell)}{\partial t} + \nabla \cdot [(\langle \mathbf{u} \rangle^i + {}^i\mathbf{u})(\langle m_\ell \rangle^i + {}^i m_\ell)] = \langle R_\ell \rangle^i + {}^i R_\ell + D_\ell \nabla^2 (\langle m_\ell \rangle^i + {}^i m_\ell) \tag{14}$$

where the mixture density $\rho$ and the coefficient $D_\ell$ in (2) have been assumed to be constant. Expanding the convection term and taking the volume average of (14) with the help of (6), one has:

$$\frac{\partial \phi \left\langle \langle m_\ell \rangle^i + {}^i m_\ell \right\rangle^i}{\partial t} + \nabla \cdot [\phi \left\langle (\langle \mathbf{u} \rangle^i \langle m_\ell \rangle^i + {}^i \mathbf{u} \langle m_\ell \rangle^i + \langle \mathbf{u} \rangle^i \, {}^i m_\ell + {}^i \mathbf{u} \, {}^i m_\ell) \right\rangle^i ] = \phi \left\langle \langle R_\ell \rangle^i + {}^i R_\ell \right\rangle^i + D_\ell \left\langle \nabla^2 \phi (\langle m_\ell \rangle^i + {}^i m_\ell) \right\rangle^i \tag{15}$$

or,

$$\frac{\partial \phi \langle m_\ell \rangle^i}{\partial t} + \nabla \cdot [\phi (\langle \mathbf{u} \rangle^i \langle m_\ell \rangle^i + \langle {}^i \mathbf{u} \, {}^i m_\ell \rangle^i)] = \phi \langle R_\ell \rangle^i + D_\ell \nabla^2 (\phi \langle m_\ell \rangle^i) \tag{16}$$

The third term on the left of (16) appears in classical analysis of mass transport in porous media (*e.g.* [2-5]) and is known as **mass dispersion**.

In order to apply the time average to (16), one defines the intrinsic volume average as:

$$\langle m_\ell \rangle^i = \overline{\langle m_\ell \rangle^i} + {\langle m_\ell \rangle^i}' \tag{17}$$

$$\langle \mathbf{u} \rangle^i = \overline{\langle \mathbf{u} \rangle^i} + {\langle \mathbf{u} \rangle^i}' \tag{18}$$

Substituting (17) and (18) in (16) and taking the time average, we obtain:

$$\frac{\partial \phi \overline{\langle m_\ell \rangle^i}}{\partial t} + \nabla \cdot \phi (\overline{\langle \mathbf{u} \rangle^i} \; \overline{\langle m_\ell \rangle^i} + \overline{{\langle \mathbf{u} \rangle^i}' {\langle m_\ell \rangle^i}'} + \overline{\langle {}^i \mathbf{u} \, {}^i m_\ell \rangle^i}) = \phi \overline{\langle R_\ell \rangle^i} + D_\ell \nabla^2 (\phi \overline{\langle m_\ell \rangle^i}) \tag{19}$$

Equation (19) is the macroscopic mass transfer equation for the species $\ell$ in the porous matrix taking first the *volume average* followed by the *time average*.

Anther route to reach a macroscopic transport equation for turbulent flow, it to invert the order of application of the same average operators applied over equation (1). Therefore, starting now with the time average, one needs to consider the time decompositions,

$$m_\ell = \overline{m}_\ell + m'_\ell \tag{20}$$

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}' \tag{21}$$

Substituting (20) and (21) into (1) one has:

$$\frac{\partial (\overline{m}_\ell + m'_\ell)}{\partial t} + \nabla \cdot [(\overline{\mathbf{u}} + \mathbf{u}')(\overline{m}_\ell + m'_\ell)] = \overline{R}_\ell + R'_\ell + D_\ell \nabla^2 (\overline{m}_\ell + m'_\ell) \tag{22}$$

where again the mixture density $\rho$ and the diffusion coefficient $D_\ell$ were kept constants. Applying time average to (22) and one obtains,

$$\overline{\frac{\partial (\overline{m}_\ell + m'_\ell)}{\partial t}} + \overline{\nabla \cdot (\overline{\mathbf{u}} \overline{m}_\ell + \overline{\mathbf{u}} m'_\ell + \mathbf{u}' \overline{m}_\ell + \mathbf{u}' m'_\ell)} = \overline{\overline{R}_\ell + R'_\ell} + D_\ell \overline{\nabla^2 (\overline{m}_\ell + m'_\ell)} \tag{23}$$

or

$$\frac{\partial \overline{m}_\ell}{\partial t} + \nabla \cdot (\overline{\mathbf{u}} \overline{m}_\ell + \overline{\mathbf{u}' m'_\ell}) = \overline{R}_\ell + D_\ell \nabla^2 \overline{m}_\ell \tag{24}$$

The second term on the left of (24) is known as **turbulent mass flux** (divided by $\rho$). It requires a model for closure of the mathematical problem.

Further, in order to apply the volume average to (24), one must first define the spatial deviations with respect to the time averages, given by:

$$\overline{m}_\ell = \langle \overline{m}_\ell \rangle^i + {}^i \overline{m}_\ell \tag{25}$$

$$\overline{\mathbf{u}} = \langle \overline{\mathbf{u}} \rangle^i + {}^i \overline{\mathbf{u}} \tag{26}$$

Substituting now (25) and (26) into (24) and performing the volume average operation, one has:

$$\frac{\partial \phi \langle \overline{m}_\ell \rangle^i}{\partial t} + \nabla \cdot \phi (\langle \overline{\mathbf{u}} \rangle^i \langle \overline{m}_\ell \rangle^i + \langle {}^i \overline{\mathbf{u}} \, {}^i \overline{m}_\ell \rangle^i + \langle \overline{\mathbf{u}' m'_\ell} \rangle^i) = \phi \langle \overline{R}_\ell \rangle^i + D_\ell \nabla^2 \phi \langle \overline{m}_\ell \rangle^i \tag{27}$$

Equation (27) is the macroscopic mass diffusion equation for the taking first the *time average* followed by the *volume average* operator.

It is interesting to observe that (27), obtained through the first procedure (*time-volume* average), is equivalent to (19) as will be shown below.

### 2.4. Application of the Double Decomposition Concept

Using now (9)-(11), the fourth term on the left hand side of (19) can be expanded as:

$$\overline{\langle {}^i\mathbf{u}\, {}^i m_\ell \rangle^i} = \overline{\langle ({}^i\overline{\mathbf{u}} + {}^i\mathbf{u}')({}^i\overline{m}_\ell + {}^i m'_\ell)\rangle^i} = \langle {}^i\overline{\mathbf{u}}\,{}^i\overline{m}_\ell\rangle^i + \overline{\langle {}^i\mathbf{u}'\, {}^i m'_\ell\rangle^i} \tag{28}$$

Substituting (28) into (19), the convection term will read,

$$\nabla\cdot(\phi\overline{\langle \mathbf{u}\; m_\ell\rangle^i}) = \nabla\cdot\{\phi(\underset{\uparrow \atop \mathbf{I}}{\overline{\langle\mathbf{u}\rangle^i}\,\overline{\langle m_\ell\rangle^i}} + \underset{\uparrow \atop \mathbf{II}}{\langle {}^i\overline{\mathbf{u}}\,{}^i\overline{m}_\ell\rangle^i} + \underset{\uparrow \atop \mathbf{III}}{\overline{\langle\mathbf{u}\rangle^{i\,\prime}\,\langle m_\ell\rangle^{i\,\prime}}} + \underset{\uparrow \atop \mathbf{IV}}{\overline{\langle {}^i\mathbf{u}'\, {}^i m'_\ell\rangle^i}})\} \tag{29}$$

Likewise, applying again (9)-(11) to the fourth term on the left hand side of (27), one gets,

$$\langle\overline{\mathbf{u}' m'_\ell}\rangle^i = \overline{\langle(\langle\mathbf{u}'\rangle^i + {}^i\mathbf{u}')(\langle m'_\ell\rangle^i + {}^i m'_\ell)\rangle^i} = \overline{\langle\mathbf{u}'\rangle^i\langle m'_\ell\rangle^i} + \overline{\langle {}^i\mathbf{u}'\; {}^i m'_\ell\rangle^i} \tag{30}$$

Also, plugging (30) into (27) will give for the same convection term,

$$\nabla\cdot(\phi\overline{\langle \mathbf{u}\; m_\ell\rangle^i}) = \nabla\cdot\{\phi(\underset{\uparrow \atop \mathbf{I}}{\langle\overline{\mathbf{u}}\rangle^i\langle\overline{m}_\ell\rangle^i} + \underset{\uparrow \atop \mathbf{II}}{\langle {}^i\overline{\mathbf{u}}\,{}^i\overline{m}_\ell\rangle^i} + \underset{\uparrow \atop \mathbf{III}}{\overline{\langle\mathbf{u}'\rangle^i\langle m'_\ell\rangle^i}} + \underset{\uparrow \atop \mathbf{IV}}{\overline{\langle {}^i\mathbf{u}'\; {}^i m'_\ell\rangle^i}})\} \tag{31}$$

Comparing (31) to (29), in light of (9), one can conclude that (27) is, in fact, equal to (19). This demonstrates that the final expanded form of the macroscopic mass transfer equation for a rigid, homogeneous porous medium saturated with an incompressible fluid does not depend on the averaging order and both procedures lead to equivalent results.

Further, the four terms on the right of either (31) or (29) could be given the following physical significance (multiplied by $\rho$):

I. **Convective Mass Flux** based on macroscopic time mean velocity and mass fraction.

II. **Mass Dispersion** associated with deviations of microscopic time mean velocity and mass fraction. Note that this term is also present when analyzing laminar mass transfer in porous media, but it does not exist if a volume averaged in not performed.

III. **Turbulent Mass Flux** due to the fluctuating components of both macroscopic velocity and mass fraction. This term is also present in turbulent flow in clear (non-porous) domains. It is not defined for laminar flow in porous media where time fluctuations do not exist.

IV. **Turbulent Mass Dispersion** in a porous medium due to both *time fluctuations* and *spatial deviations* of both microscopic velocity and mass fraction.

Thus, the macroscopic mass transport equation for an incompressible flow in a rigid, homogeneous and saturated porous medium can be written as:

$$\frac{\partial\phi\langle\overline{m}_\ell\rangle^i}{\partial t} + \nabla\cdot\phi(\langle\overline{\mathbf{u}}\rangle^i\langle\overline{m}_\ell\rangle^i + \langle {}^i\overline{\mathbf{u}}\;{}^i\overline{m}_\ell\rangle^i + \overline{\langle\mathbf{u}'\rangle^i\langle m'_\ell\rangle} + \overline{\langle {}^i\mathbf{u}'\;{}^i m'_\ell\rangle^i}) = \phi\langle\overline{R}_\ell\rangle^i + D_\ell\nabla^2(\phi\langle\overline{m}_\ell\rangle^i) \tag{32}$$

or in its equivalent form (see (9) ),

$$\frac{\partial\phi\overline{\langle m_\ell\rangle^i}}{\partial t} + \nabla\cdot\phi(\overline{\langle\mathbf{u}\rangle^i}\,\overline{\langle m_\ell\rangle^i} + \langle {}^i\overline{\mathbf{u}}\;{}^i\overline{m}_\ell\rangle^i + \overline{\langle\mathbf{u}\rangle^{i\,\prime}\langle m_\ell\rangle^{i\,\prime}} + \overline{\langle {}^i\mathbf{u}'\;{}^i m'_\ell\rangle^i}) = \phi\overline{\langle R_\ell\rangle^i} + D_\ell\nabla^2(\phi\overline{\langle m_\ell\rangle^i}) \tag{33}$$

### 2.5. Macroscopic Turbulent Model for Mass Transfer

All terms in (32) or (33) need to be represented or modeled as functions of the macroscopic mass fraction $\langle\overline{m}_\ell\rangle^i$. Using gradient type diffusion models, the proposed forms for the different mechanisms are as follows:

**Mass Dispersion**: Following the literature [2-5], a time-mean version for a dispersion model is given as,

$$\rho\langle {}^i\overline{\mathbf{u}}\;{}^i\overline{m}_\ell\rangle^i = \rho\,\mathbf{D}_{disp}\nabla.\langle\overline{m}_\ell\rangle^i \tag{34}$$

where the dispersion coefficient $\mathbf{D}_{disp}$ is a second order tensor.

**Turbulent Mass Flux**:

$$-\rho\,\overline{\langle\mathbf{u}'\rangle^i\langle m'_\ell\rangle^i} = -\rho\,\overline{\langle\mathbf{u}\rangle^{i\,\prime}\,\langle m_\ell\rangle^{i\,\prime}} = \rho\,\mathbf{D}_t\cdot\nabla\langle\overline{m}_\ell\rangle^i \tag{35}$$

**Turbulent Mass Dispersion**:

$$-\rho\langle \overline{{}^{i}\mathbf{u}'\,{}^{i}m'_{\ell}}\rangle^{i} = \rho\,\mathbf{D}_{disp,t}\cdot\nabla\langle\overline{m}_{\ell}\rangle^{i} \tag{36}$$

The coefficients $\mathbf{D}_{t}$ and $\mathbf{D}_{disp,t}$ in equation (35) and (36), respectively, will be combined as suggested above by equation (30). Therefore, the two additional transport mechanisms, namely the *turbulent mass flux* and *turbulent mass dispersion*, can be added up so that a model for $\langle\overline{\mathbf{u}'m'_{\ell}}\rangle^{i}$ will be necessary for closure of the mathematical problem.

Starting out from the time averaged mass transfer equation coupled with the microscopic modeling for the *turbulent mass flux vector* through the microscopic Eddy diffusivity, $D_{\ell,t} = \dfrac{\mu_t}{\rho\, Sc_{\ell,t}}$, one can write:

$$-\rho\overline{\mathbf{u}'m'_{\ell}} = \rho D_{\ell.t}\,\nabla\overline{m}_{\ell} = \frac{\mu_t}{Sc_{\ell,t}}\nabla\overline{m}_{\ell} \tag{37}$$

where the microscopic Eddy Viscosity in (37), $\mu_t$, is given by:

$$\mu_t = \rho\, c_{\mu}\,\frac{k^2}{\varepsilon} \tag{38}$$

and $Sc_{\ell,t}$ is the turbulent Schmidt number for the species $\ell$, which is taken here as a constant. Also $k$ and $\varepsilon$ are the turbulent kinetic energy and its dissipation rate, respectively.

Applying the volume average to the resulting equation, one obtains the macroscopic turbulent mass flux vector, given by:

$$-\rho\langle\overline{\mathbf{u}'m'_{\ell}}\rangle^{i} = \rho\langle D_{\ell.t}\rangle^{i}\,\nabla\langle\overline{m}_{\ell}\rangle^{i} = \rho\,(\mathbf{D}_{t}+\mathbf{D}_{disp,t})\cdot\nabla\langle\overline{m}_{\ell}\rangle^{i} = \frac{\mu_{t_\phi}}{Sc_{\ell,t}}\nabla\langle\overline{m}_{\ell}\rangle^{i} \tag{39}$$

where the symbol $\mu_{t_\phi}$ expresses the macroscopic version of the Eddy viscosity, given by:

$$\mu_{t_\phi} = \rho\, c_{\mu}\,\frac{\langle k\rangle^{i\,2}}{\langle\varepsilon\rangle^{i}} \tag{40}$$

A mentioned above, in light of equations (30) and (39) the overall macroscopic mass flux due to turbulence is taken as the sum of the turbulent mass flux and the turbulent mass dispersion appearing in either (31) or (29). Further, the isotropic nature of expression (40) suggests the equality,

$$\mathbf{D}_{t}+\mathbf{D}_{disp,t} = \frac{1}{\rho}\frac{\mu_{t_\phi}}{Sc_{\ell,t}}\mathbf{I} \tag{41}$$

Likewise, a constant value for the molecular diffusion coefficient in (2) leads to a macroscopic diffusion coefficient, $\mathbf{D}_{diff}$, of the form,

$$\mathbf{D}_{diff} = \langle D_{\ell}\rangle^{i}\,\mathbf{I} = \frac{1}{\rho}\frac{\mu_{\phi}}{Sc_{\ell}}\mathbf{I} \tag{42}$$

Finally, using the Dupuit-Forchheimer relationship, $\mathbf{u}_D = \langle\overline{\mathbf{u}}\rangle^{v} = \phi\langle\overline{\mathbf{u}}\rangle^{i}$, in combination with (34), (42) and (41), the final modeled form for a transport equation can be written as,

$$\frac{\partial\phi\,\langle\overline{m}_{\ell}\rangle^{i}}{\partial t} + \nabla\cdot(\overline{\mathbf{u}}_{D}\,\langle\overline{m}_{\ell}\rangle^{i}) = \nabla\cdot\mathbf{D}_{eff}\cdot\nabla(\phi\langle\overline{m}_{\ell}\rangle^{i}) + \phi\langle\overline{R}_{\ell}\rangle^{i}$$

where

$$\mathbf{D}_{eff} = \mathbf{D}_{disp}+\mathbf{D}_{diff}+\mathbf{D}_{t}+\mathbf{D}_{disp,t} = \mathbf{D}_{disp}+\frac{1}{\rho}\left(\frac{\mu_{\phi}}{Sc_{\ell}}+\frac{\mu_{t_\phi}}{Sc_{\ell,t}}\right)\mathbf{I} = \mathbf{D}_{disp}+\frac{1}{\rho}\left(\frac{\mu_{\phi,ef}}{Sc_{\ell,ef}}\right)\mathbf{I} \tag{43}$$

In (42), $Sc_{\ell,ef}$ is the Effective Macroscopic Turbulent Schmidt number given by,

$$Sc_{\ell,ef} = \frac{\mu_{ef_\phi}}{\frac{\mu_\phi}{Sc_\ell} + \frac{\mu_{t_\phi}}{Sc_{\ell,t}}} \tag{44}$$

### 3. Numerical Determination of Dispersion Coefficients

In order to calculate the dispersion coefficients in equation (34), a methodology is here described. For the steady Laminar and Turbulent flow regimes, we shall consider a macroscopically uniform flow with an angle $\theta$ meandering through an infinite number of cylinders rods placed in a regular fashion, as illustrated in Fig.3. Thus, the macroscopic velocity field follows:

$$\langle \overline{\mathbf{u}} \rangle^v = \left| \langle \overline{\mathbf{u}} \rangle^v \right| \left( \cos\theta \, \vec{i} + \sin\theta \, \vec{j} \right) \tag{45}$$

Two distinct macroscopic mass fraction fields are considered to obtain the transverse and longitudinal dispersions. First, we impose a macroscopically linear mass fraction gradient perpendicularly to macroscopic flow direction, in the form,

$$\nabla \langle \overline{m_l} \rangle = \frac{\Delta m_l}{H} (-\sin\theta \, \vec{i} + \cos\theta \, \vec{j}) \text{ : Transverse dispersion} \tag{46}$$

to determine transverse mass fraction dispersion, and a macroscopically linear mass fraction gradient parallel to the main flow, such as,

$$\nabla \langle \overline{m_l} \rangle = \frac{\Delta m_l}{H} (\cos\theta \, \vec{i} + \sin\theta \, \vec{j}) \text{ ; Longitudinal dispersion} \tag{47}$$

to determine the longitudinal mass fraction dispersion.

The boundary, compatibility and periodic constraints are given as follows:

**On the periodic boundaries**:

$$\begin{aligned} \overline{\mathbf{u}}\big|_{x=0} &= \overline{\mathbf{u}}\big|_{x=H} \\ \overline{\mathbf{u}}\big|_{y=0} &= \overline{\mathbf{u}}\big|_{y=H} \end{aligned} \tag{48}$$

$$\begin{aligned} \left. \int_0^H \overline{u} \, dy \right|_{x=0} &= \left. \int_0^H \overline{u} \, dy \right|_{x=H} = H \left| \langle \overline{\mathbf{u}} \rangle^v \right| \cos\theta \\ \left. \int_0^H \overline{v} \, dx \right|_{y=0} &= \left. \int_0^H \overline{v} \, dx \right|_{y=H} = H \left| \langle \overline{\mathbf{u}} \rangle^v \right| \sin\theta \end{aligned} \tag{49}$$

For the mass fraction boundary conditions, we impose

$$\begin{aligned} m_l\big|_{x=0} &= m_l\big|_{x=H} + \Delta T \sin\theta \\ m_l\big|_{y=0} &= m_l\big|_{y=H} - \Delta T \cos\theta \end{aligned} \tag{50}$$

as we determine the transversal mass fraction dispersion, and

$$\begin{aligned} m_l\big|_{x=0} &= m_l\big|_{x=H} - \Delta T \cos\theta \\ m_l\big|_{y=0} &= m_{l\,y=H} - \Delta T \sin\theta \end{aligned} \tag{51}$$

as we determine the longitudinal mass fraction dispersion.

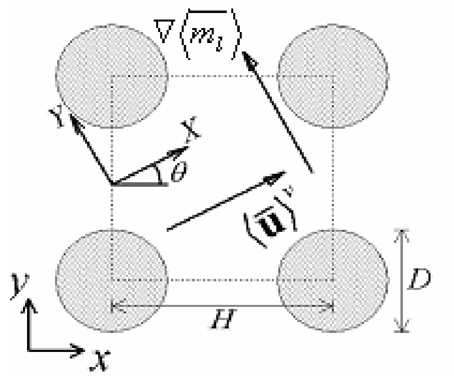


Figure 3 – Physical model and its coordinate system

Following references [7]and [8], we integrate the microscopic mass equation (1) for the incompressible fluid over a *REV (*see Fig.1), and obtain,

$$\rho\left[\frac{1}{V}\int_{A_{int}}\left(\overline{m_l}-\langle\overline{m_l}\rangle^i\right)\left(\overline{\mathbf{u}}-\langle\overline{\mathbf{u}}\rangle^i\right)d\vec{A}\right]=\rho D_{disp}\frac{1}{V}\int_{A_{int}}\nabla\left(\overline{m_l}\right)d\vec{A} \tag{52}$$

where $A_{int}$ is the total area in the fluid phase within a control volume $V$, while $dA$ is its vector element pointing outward from the fluid side to solid side.

The diffusivities tensor components $D_{xx}$ and $D_{yy}$ are introduced to model the mass dispersion, by a gradient-type diffusion hypothesis. In this study , we shall determine the dispersion conductively purely from the theoretical basis by substituting the microscopic results into (34).

Let us set one coordinate along the macroscopic flow direction. Then, only diagonal components of the mass dispersion tensors remain non-zero components, when the macroscopically linear mass fraction gradient is impose along the $X$ direction and the $Y$ direction normal of the macroscopic flow. The YY components of $D_{disp}$ can readily be determined from

$$D_{disp\,YY}=\frac{\frac{1}{H^2}}{\left(\Delta m_l/H\right)}\int_0^H\int_0^H\left(\overline{m_l}-\langle\overline{m_l}\rangle^i\right)\left(\overline{\mathbf{u}}-\langle\overline{\mathbf{u}}\rangle^i\right)dxdy\left(-\sin\theta\,\vec{\mathrm{i}}+\cos\theta\,\vec{\mathrm{j}}\right) \tag{53}$$

Similarly, when the macroscopically linear mass fraction gradient is imposed along the $X$ direction of the macroscopic flow, the $XX$ components of $D_{disp}$ can readily be determined from

$$D_{disp\,XX}=\frac{\frac{1}{H^2}}{\left(\Delta m_l/H\right)}\int_0^H\int_0^H\left(\overline{m_l}-\langle\overline{m_l}\rangle^i\right)\left(\overline{\mathbf{u}}-\langle\overline{\mathbf{u}}\rangle^i\right)dxdy\left(\cos\theta\,\vec{\mathrm{i}}+\sin\theta\,\vec{\mathrm{j}}\right) \tag{54}$$

## 4. Conclusions

In this work it was shown that, under the light of the double decomposition concept [14, 15], both procedures employed to arrive at the macroscopic mass transfer equation, namely *time-volume averaging* or *volume-time averaging*, lead to the same result for the case of incompressible flow in a rigid, homogeneous porous medium. The extra terms appearing in equation still need to be modeled in terms of $\overline{\mathbf{u}}_D$ and $\langle\overline{m}_\ell\rangle^i$. It is expected that additional research on this new subject be stimulated by the derivations here presented.

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