

NUMERICAL DETERMINATION OF TRANSVERSE MASS DISPERSION COEFFICIENTS IN POROUS MEDIA

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Abstract. Mass dispersion in porous media is an import phenomenon and its study has applications in combustion and in steam injection systems for Enhanced Oil Recovery, for example. Accordingly, the study of flow through porous media has gained much attention lately and advances in proper modelling of such flows, which include non-linear effects, have been published. In this work, mass dispersion tensors were calculated within an infinite porous medium formed by spatially periodic array of longitudinally-displaced square and ellipticals rods. For the sake of simplicity, just one unit-cell, together with periodic boundary conditions for mass and momentum equations, and Neumann conditions for the mass concentration, was used to represent such medium. The numerical methodology employed is based on the control volume approach. Turbulence is assumed to exist within the fluid phase and High- as well as Low-Reynolds $k-\epsilon$ models are used to model such non-linear effects. The flow equations at the pore-scale were numerically solved using the SIMPLE method on non-orthogonal boundary-fitted coordinate system. Dispersion coefficients are obtained by integrating the distributed parameters within the unit cell.

Keywords: Porous media, Mass Dispersion, Turbulence, Numerical Methods

1. Introduction

Due to its great application in industry and science, the study of the flow in porous media has received great attention lately and advances in proper modeling of such flows, including non-linear effects, have been published (Pedras and de Lemos, 2001a; de Lemos and Pedras, 2001; Rocamora and de Lemos, 2000; Pedras and de Lemos, 2001b; Pedras and de Lemos, 2001c; Pedras et al., 2003; Pedras and de Lemos, 2003). Engineering systems based on fluidized bed combustion, enhanced oil reservoir recovery, combustion in an inert porous matrix, underground spreading of chemical waste and chemical catalytic reactors are just a few examples of such applications. In some of these applications the thermal dispersion in porous media is an important phenomenon, in which one has used (Hsu and Cheng, 1990; Kaviani, 1995; Ochoa-Tapia and Whitaker, 1997; Moyne, 1997; Quintard et al., 1997; Kuwahara and Nakayama, 1998; Nakayama and Kuwahara, 1999) the notion of a Representative Elementary Volume (REV, Fig.1) for the mathematical treatment of governing equations. These models, based on the macroscopic point of view, lose details on the flow pattern inside the REV and, together with ad-hoc information, provide global flow properties such as average velocities and temperatures.

Such flows can also be analyzed by modeling the topology of the porous medium and resolving the flow equations at the pore-scale. This treatment reveals the flow structure at the pore-scale level and was used by (Quintard et al., 1997; Kuwahara and Nakayama, 1998; Nakayama and Kuwahara, 1999; Rocamora and de Lemos, 2002) to calculate the thermal dispersion tensors and (De-Lemos e Mesquita (2003) and De-Lemos e Mesquita (2003)a) to calculate the mass dispersion tensors with periodic boundary condition for the mass, momentum and the energy equations.

The aim of the present contribution is to discuss the modeling of mass dispersion and calculate the mass dispersion tensors within an infinite porous medium formed by spatially periodic array of longitudinally-displaced cylindrical rods. For the sake of simplicity, just one unit-cell, together with periodic boundary conditions for mass and momentum equations, and Neumann conditions for the mass fraction equation, was used to represent such medium. Turbulence is assumed to exist within the fluid phase and a high and a Low Reynolds $k-\epsilon$ models are used to model such non-linear effects.

The flow equations at the pore-scale were numerically solved using the SIMPLE method on a non-orthogonal boundary-fitted coordinate system. The integrated results were compared to the existing data presented in the literature.

2. Microscopic equations

The following microscopic transport equations describe the flow field and the Mass transfer process within a porous medium, where barred quantities represent time-averaged components and primes indicate turbulent fluctuations:

$$\nabla \cdot \bar{\mathbf{u}}$$

(1)

$$\rho \left[\frac{\partial \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\mathbf{u}} \bar{\mathbf{u}}) \right] = -\nabla \bar{p} + \nabla \cdot \{ \mu [\nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^T] - \rho \overline{\mathbf{u}' \mathbf{u}'} \} \quad (2)$$

$$\frac{\partial \bar{m}_\ell}{\partial t} + \nabla \cdot (\rho_f \bar{\mathbf{u}} \bar{m}_\ell) = \bar{R}_\ell + D_\ell \nabla^2 (\bar{m}_\ell) \quad (3)$$

$$\rho \left[\frac{\partial k}{\partial t} + \nabla \cdot (\bar{\mathbf{u}} k) \right] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] - \rho \overline{\mathbf{u}' \mathbf{u}'} : \nabla \bar{\mathbf{u}} - \rho \varepsilon \quad (4)$$

$$\rho \left[\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\bar{\mathbf{u}} \varepsilon) \right] = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + [c_1 (-\rho \overline{\mathbf{u}' \mathbf{u}'} : \nabla \bar{\mathbf{u}}) - c_2 f_2 \rho \varepsilon] \frac{\varepsilon}{k} \quad (5)$$

$$-\rho \overline{\mathbf{u}' \mathbf{u}'} = \mu_t [\nabla \bar{\mathbf{u}} + (\nabla \bar{\mathbf{u}})^T] - \frac{2}{3} \rho k \mathbf{I} \quad (6)$$

$$-\rho \overline{\mathbf{u}' m'_\ell} = \rho D_{\ell,t} \nabla \bar{m}_\ell = \frac{\mu_t}{Sc_{\ell,t}} \nabla \bar{m}_\ell \quad (7)$$

$$\mu_t = \rho \nu_t = \rho c_\mu f_\mu \frac{k^2}{\varepsilon} \quad (8)$$

where $\mathbf{u}$ is the microscopic velocity, ρ is the bulk density of the mixture, p the thermodynamic pressure, μ and μ_t the dynamic and turbulent viscosities, m_ℓ is the mass fraction of component ℓ , D_ℓ is the diffusion coefficient of species ℓ , k the turbulent kinetic energy and ε the dissipation of k . In the equations σ_k and σ_ε are effective Prandtl numbers, Sc_ℓ is the Schmidt number for the species ℓ , c_1 , c_2 and c_μ are dimensionless constants and f_2 and f_μ damping functions.

In this work the use of the low Re k- ε model is justified by the fact that the turbulent flow in porous media occurs for Reynolds numbers (based on the pore) relatively low. To account for the low Reynolds effects, the following damping functions and model constants were adopted (Abe et al., 1992):

$$f_2 = \left\{ 1 - \exp \left[- \frac{(\nu \varepsilon)^{0.25} n}{3.1 \nu} \right] \right\}^2 \times \left\{ 1 - 0.3 \exp \left[- \left(\frac{k^2 / \nu \varepsilon}{6.5} \right)^2 \right] \right\} \quad (9)$$

$$f_\mu = \left\{ 1 - \exp \left[- \frac{(\nu \varepsilon)^{0.25} n}{14 \nu} \right] \right\}^2 \times \left\{ 1 + \frac{5}{(k^2 / \nu \varepsilon)^{0.75}} \exp \left[- \left(\frac{k^2 / \nu \varepsilon}{200} \right)^2 \right] \right\} \quad (10)$$

$$c_\mu = 0.09, \quad c_1 = 1.5, \quad c_2 = 1.9, \quad \sigma_k = 1.4, \quad \sigma_\varepsilon = 1.3, \quad \sigma_{m_\ell} = 0.7. \quad (11)$$

For the unit-cell represented in Fig.(4) and with the assumption of macroscopic fully developed uni-dimensional flow, the boundary conditions are given as follow:

At the walls:

$$\bar{\mathbf{u}} = 0; \bar{m}_\ell = 0; k = 0 \text{ and } \varepsilon = \nu \frac{\partial^2 k}{\partial n^2} \quad (12)$$

On $x=0$ and $x=H$ periodic boundaries (momentum equation),

$$\bar{\mathbf{u}}|_{x=0} = \bar{\mathbf{u}}|_{x=H}, \bar{\mathbf{v}}|_{x=0} = \bar{\mathbf{v}}|_{x=H}, k|_{x=0} = k|_{x=H}, \varepsilon|_{x=0} = \varepsilon|_{x=H} \quad (13)$$

On $y=0$ and $y=H$,

$$\frac{\partial \bar{u}}{\partial y} = \frac{\partial \bar{v}}{\partial y} = \frac{\partial k}{\partial y} = \frac{\partial \varepsilon}{\partial y} = 0 \quad (14)$$

The mass fraction boundary conditions will be presented in the next section. The Figures (2) and (3) shows the set of meshes used for the solutions of the problem.

3. Mass dispersion modeling

Using the double decomposition concept (Pedras and de Lemos 2001a) of a general quantity φ ,

$$\varphi = \langle \bar{\varphi} \rangle + {}^i \bar{\varphi} + \langle \varphi' \rangle + {}^i \varphi' \quad (15)$$

and following the procedure of Rocamora and de Lemos 2000 and Rocamora and de Lemos 2002, the volume averaging of the mass fraction equation (3) over the REV, renders:

$$\frac{\partial \phi \langle \bar{m}_\ell \rangle^i}{\partial t} + \nabla \cdot (\bar{\mathbf{u}}_D \langle \bar{m}_\ell \rangle^i) = \nabla \cdot \mathbf{D}_{eff} \cdot \nabla (\phi \langle \bar{m}_\ell \rangle^i) + \phi \langle \bar{R}_\ell \rangle^i \quad (16)$$

where $\langle \varphi \rangle$ is the volume average of φ , $\langle \varphi \rangle^i$ the intrinsic average of φ , φ' the time fluctuation of φ , ${}^i \varphi$ the space deviation of φ . The effective Dispersion, D_{eff} , and the dispersion tensor, D_{disp} , are defined as:

$$\mathbf{D}_{eff} = \mathbf{D}_{disp} + \mathbf{D}_{diff} + \mathbf{D}_t + \mathbf{D}_{disp,t} = \mathbf{D}_{disp} + \frac{1}{\rho} \left(\frac{\mu_\phi}{Sc_\ell} + \frac{\mu_{t,\phi}}{Sc_{t,\ell}} \right) \mathbf{I} = \mathbf{D}_{disp} + \frac{1}{\rho} \left(\frac{\mu_{\phi,ef}}{Sc_{\ell,ef}} \right) \mathbf{I} \quad (17)$$

$$-\rho \left\langle {}^{i-i} \mathbf{u} \bar{m}_\ell \right\rangle^i = \rho \mathbf{D}_{disp} \nabla \cdot \langle \bar{m}_\ell \rangle \quad (18)$$

In order to calculate the dispersion coefficients in equation (18), a methodology is here described. For the steady Laminar and Turbulent flow regimes, we shall consider a macroscopically uniform flow meandering through an infinite number of cylinders rods placed in a regular fashion. Thus, the macroscopic velocity and mass fraction fields are given by

$$\langle \bar{\mathbf{u}} \rangle^v = \left| \langle \bar{\mathbf{u}} \rangle^v \right| (\cos \theta \vec{i} + \sin \theta \vec{j}) \quad (19)$$

$$\nabla \langle \bar{m}_\ell \rangle = \frac{\Delta m_\ell}{H} (-\sin \theta \vec{i} + \cos \theta \vec{j}) \quad (20)$$

$$\nabla \langle \bar{m}_\ell \rangle = \frac{\Delta m_\ell}{H} (\cos \theta \vec{i} + \sin \theta \vec{j}) \quad (21)$$

Two distinct macroscopic mass fraction fields are considered to obtain the transverse and longitudinal dispersions. First, we impose a macroscopically linear mass fraction gradient, $\Delta \langle \bar{m}_\ell \rangle_x$, perpendicularly to macroscopic flow direction (see Fig 4 a), in the form to determine transverse mass fraction dispersion, and a macroscopically linear mass fraction gradient, $\Delta \langle \bar{m}_\ell \rangle_y$, parallel to the main flow (see Fig. 4 b).

In those cases $\Delta \langle \bar{m}_\ell \rangle_x$ and $\Delta \langle \bar{m}_\ell \rangle_y$ are no longer given values, but rather a consequence of the imposed mass fluxes at the north and south boundaries, Their values is then calculates as,

$$\Delta \langle \bar{m}_\ell \rangle_x = \frac{1}{H} \int_{y=0}^{y=H} [\bar{m}_{\ell,x=H} - \bar{m}_{\ell,x=0}] dy \quad (22)$$

As we determine the transversal mass fraction dispersion, and

$$\Delta \langle \overline{m_\ell} \rangle_y = \frac{1}{H} \int_{x=0}^{x=H} \left[\overline{m_\ell}_{y=H} - \overline{m_\ell}_{y=0} \right] dx \quad (23)$$

As we determine the longitudinal mass fraction dispersion.

Following Kuwahara and Nakayama, we integrate the microscopic mass equation (3) for the incompressible fluid over a *REV* (see Fig.1), and obtain,

$$\rho \left[\frac{1}{V} \int_{A_{int}} \left(\overline{m_\ell} - \langle \overline{m_\ell} \rangle \right) \left(\overline{\mathbf{u}} - \langle \overline{\mathbf{u}} \rangle \right) d\vec{A} \right] = \rho D_{disp} \frac{1}{V} \int_{A_{int}} \nabla (\overline{m_\ell}) d\vec{A} \quad (24)$$

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

The diffusivities tensor components $D_{disp,xx}$ and $D_{disp,yy}$ 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 (18).

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

$$(D_{disp})_{YY} = \frac{-\frac{1}{H^2} \int_0^H \int_0^H \left(\overline{m_\ell} - \langle \overline{m_\ell} \rangle \right) \left(\overline{\mathbf{u}} - \langle \overline{\mathbf{u}} \rangle \right) \cdot (-\sin \theta \vec{i} + \cos \theta \vec{j}) dx dy}{\left(\frac{\Delta \langle \overline{m_\ell} \rangle_y}{H} \right)} \quad (25)$$

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

$$(D_{disp})_{XX} = \frac{-\frac{1}{H^2} \int_0^H \int_0^H \left(\overline{m_\ell} - \langle \overline{m_\ell} \rangle \right) \left(\overline{\mathbf{u}} - \langle \overline{\mathbf{u}} \rangle \right) \cdot (\cos \theta \vec{i} + \sin \theta \vec{j}) dx dy}{\left(\frac{\Delta \langle \overline{m_\ell} \rangle_x}{H} \right)} \quad (26)$$

4. Numerical model

The governing equations were discretized using the finite volume procedure, Patankar 1980. The SIMPLE algorithm for the pressure-velocity coupling was adopted to correct both the pressure and the velocity fields. The process starts with the solution of the two momentum equations. Then the velocity field is adjusted in order to satisfy the continuity principle. This adjustment is obtained by solving the pressure correction equation. After that, the turbulence model equations and the energy equation are relaxed to update the k , ε and mass fraction fields. Details on the numerical discretization can be found in Pedras and de Lemos 2001b.

5. Results and discussion

A total of forty eight runs were carried out being thirty for laminar flow and eighteen for turbulent flow with High and low Reynolds model theory for the case which was used square rods and for the elliptical rods a total of eighty four runs carried out being sixty nine for laminar flow and fifteen for turbulent flow (six runs were used high Reynolds turbulent model and nine low Reynolds turbulent model). In all runs it was used for the fluid phase Schmidt number of 1.0 and a diffusion coefficient of species ℓ , $D_\ell = 1.455e-5 \text{ m}^2 / \text{s}$.

The transverse component of the mass dispersion tensor are show in Figure 6 as a function of Peclet Number for different porosities (for $\phi = 0.65$, $\phi = 0.75$ and $\phi = 0.90$). As can be observed, for the calculated lateral dispersion coefficients are good agreements with experimental values, in the case, was used the square model for the REV (see Figure 5), within square rods. Figure 7 shows the transverse component of the mass dispersion as an function of Peclet Number for following values of porosities (for $\phi = 0.60$, $\phi = 0.75$ and $\phi = 0.90$). In this case, for the calculated lateral dispersion coefficients are not good agreements with experimental values. The probable reason for this behavior this, are associate to the fact of the real porous medium there are local heterogeneities that must generate a much larger lateral motion, which in turn is responsible for the lateral dispersion coefficients observed in experimental works.

Finally, the Figures 8, 9, 10 and 11 shows the mass concentrations fields for dieferents values of Reynolds numbers. The mass concentration was calculated with the boundary conditions skekthed in Figure 4. as the flow rate increases, the fluid mass concetration becomes more homogeneous due to enhancement of the convection strengh.

6. Acknowledgements

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7. References

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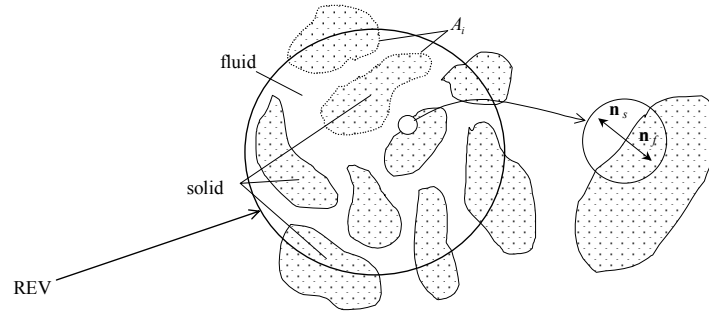


Figure 1 : Representative elementary volume (REV).

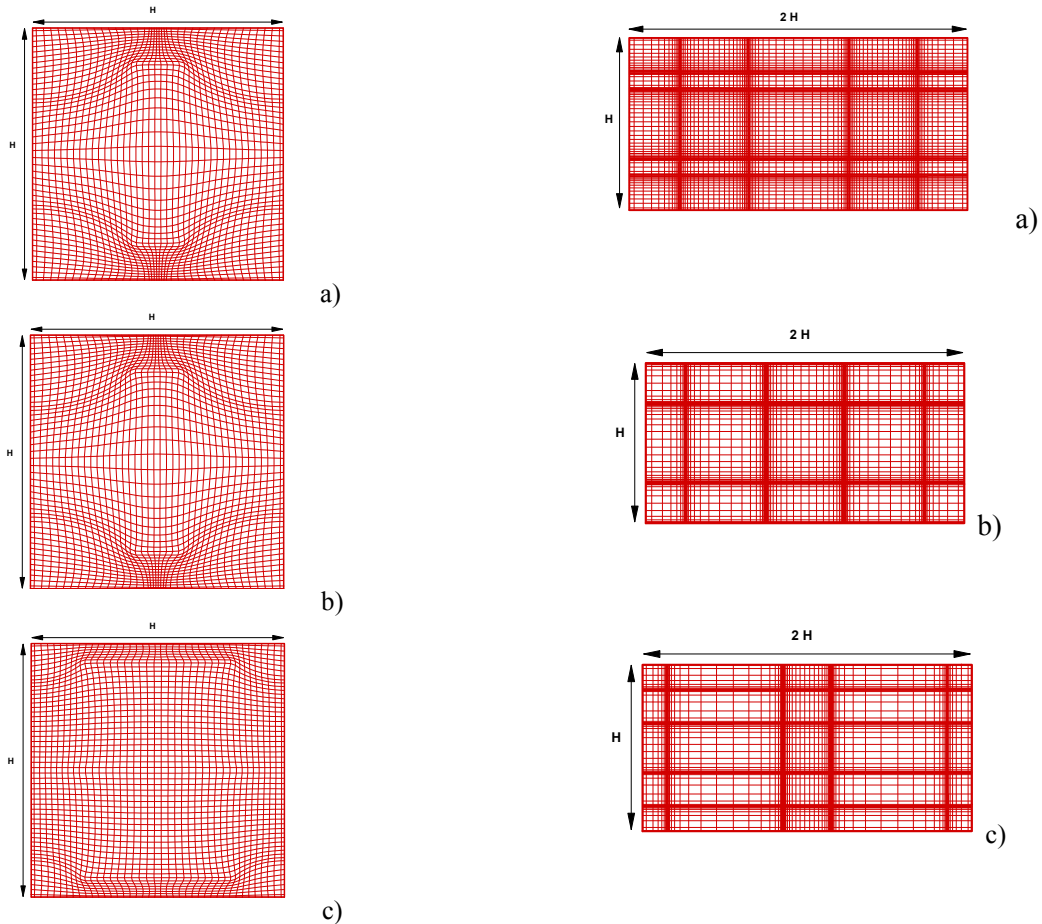


Figure 2 – Algebraically generated grids for elliptical rods: a) $\phi = 0.60$, b) $\phi = 0.75$ and c) $\phi = 0.90$

Figure 3: Algebraically generated grid for square rods: a) $\phi = 0.65$ b) $\phi = 0.75$ and c) $\phi = 0.90$.

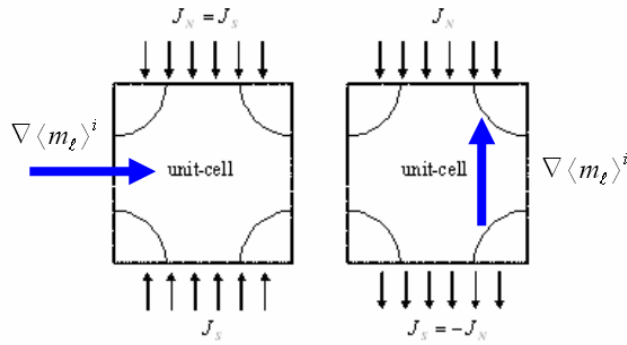


Figure 4 - Neumann boundary conditions for the mass fraction. from left to right. longitudinal gradient and transversal gradient. respectively.

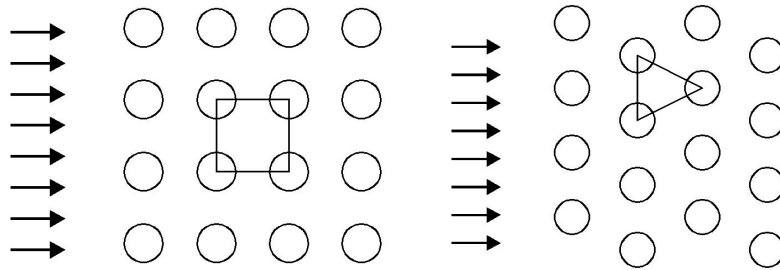


Figure 5 – Square and staggered models for the REV.

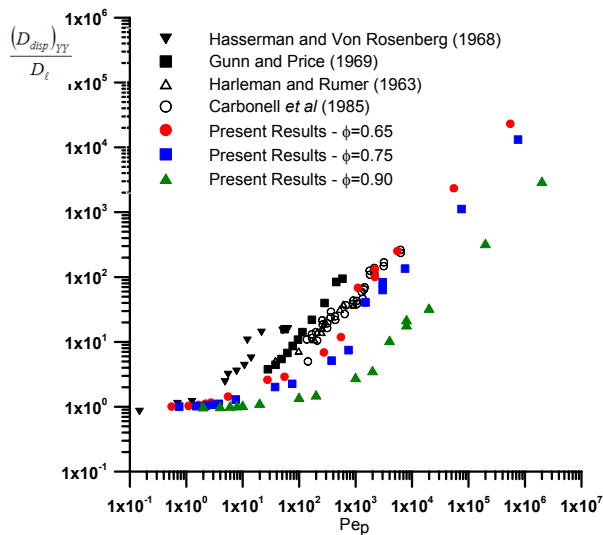


Figure 6: Transverse Mass Dispersion – Square rods.

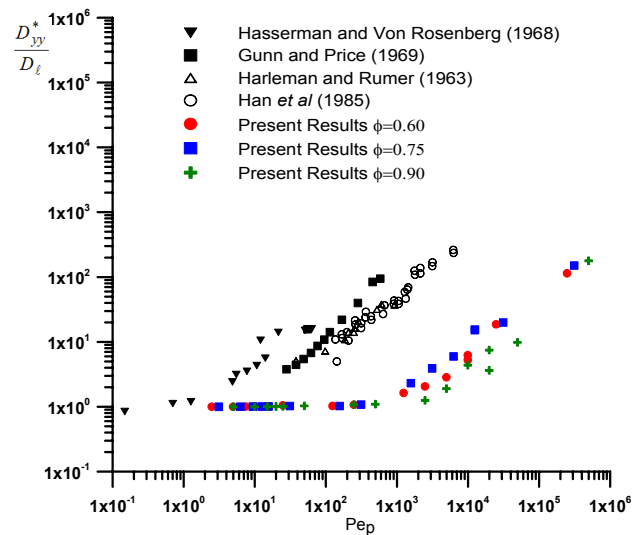
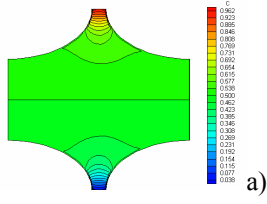
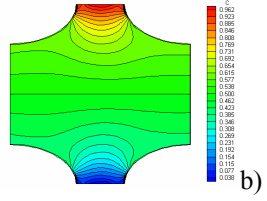


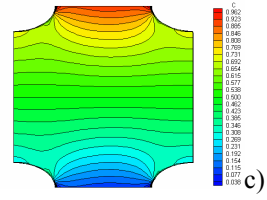
Figure 7 – Transverse Mass Dispersion – Elliptical rods.



a)

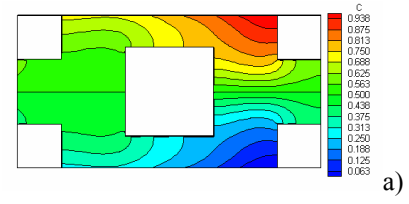


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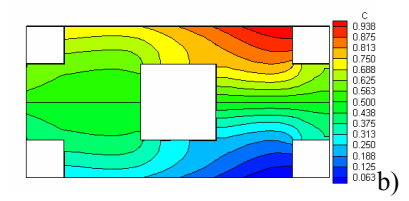


c)

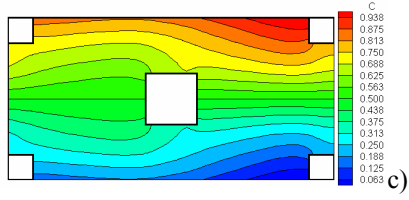
Figure 8 - Mass concentration – (Laminar regime - $Re_H = 1.0$) a) $\phi = 0.60$, b) $\phi = 0.75$ and c) $\phi = 0.90$.



a)

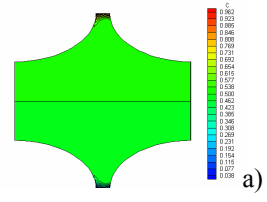


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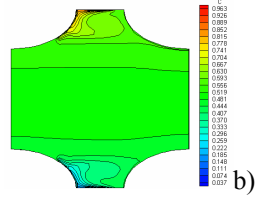


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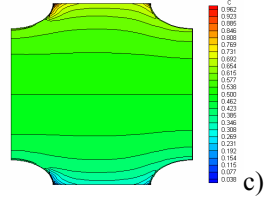
Figure 9 - Mass concentration – (Laminar regime - $Re_H = 1.0E+01$) a) $\phi = 0.65$, b) $\phi = 0.75$ and c) $\phi = 0.90$.



a)

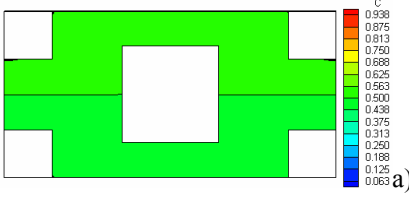


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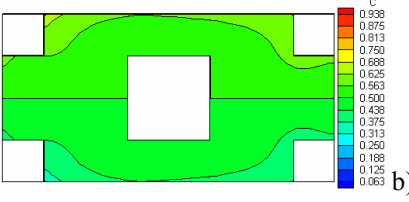


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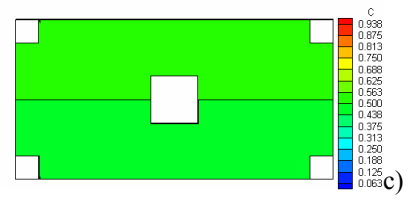
Figure 10 - Mass concentration fields (Turbulent regime – Low Reynolds model - $Re_H = 4.0E+03$): a) $\phi = 0.60$, b) $\phi = 0.80$ and c) $\phi = 0.90$.



a)



b)



c)

Figure 11 - Mass concentration fields (Turbulent regime – High Reynolds model - $Re_H = 1.0E+06$): a) $\phi = 0.65$, b) $\phi = 0.80$ and c) $\phi = 0.90$.