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The Effect of the Dispersion Term on Flux of a Fluid in Permeable Media

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Abstract:
The flux of a fluid in permeable media can be modelled using a continuous or a multi-continuous. To link the real system with the continuous model is mandatory to realize a suitable average of the equations and of the variables governed by them. The dispersion term comes from this averaging but it is not only a mathematical product of the modelling. It take in account of an important phenomenon that is similar to diffusion but that differs from it because not depends from molecular excitement. The dispersion is due to the intrinsic geometry of the permeable media that forces the real paths of the flux to divert from the average one. In this work a model of the dispersion term is evaluated and the results are compared with the corresponding cases without it. Granular permeable media is considered with a compressible flux. The PDE module of COMSOL is utilized.

Keywords: dispersion, permeable, porous, fluid, flow

1 Introduction

A robust and rigorous method to model the flow in a permeable media is based on the average of the flow equations. The average is computed on a Reference Elementary Volume. It must be a small volume (ideally infinitesimal) if compared with the permeable media domain and it must be large if compared with the pore-scale of the permeable media so that when it move a quantity changes not abruptly. The REV is of crucial importance to build (and also to test) a continuous model of flow in permeable media. The volume average of a some quantity defined in the void part of the permeable media, is computed as follows

$$\langle \eta \rangle = \frac{1}{V_0} \int_{\Omega_0} \eta \, dV \tag{1}$$

Where Ω_0 is the REV and V_0 is its measure.
For the intrinsic average $\langle . \rangle^i$, i.e. that computed only on the void portion of the REV, is valid the following equation

$$\langle \eta \rangle = \varepsilon \langle \eta \rangle^i \tag{2}$$

Where $\varepsilon = V_{void}/V_0$ is the porosity.
Moreover the spatial deviation is defined as follows

$$\eta^{\ominus} = \eta - \langle \eta \rangle^i \tag{3}$$

The aforesaid volumetric average of the flow equations can be obtained, as reported in [1], by mean of the Theorem of Local Volumetric Average. The following equations are deduced from this theorem.

$$\langle \nabla \eta \rangle = \nabla(\varepsilon \langle \eta \rangle^i) + \frac{1}{V_0} \int_{\mathcal{A}_i} \mathbf{n}_i \, \eta \, dS \tag{4}$$

$$\langle \nabla \cdot \mathbf{w} \rangle = \nabla \cdot (\varepsilon \langle \mathbf{w} \rangle^i) + \frac{1}{V_0} \int_{\mathcal{A}_i} \mathbf{n}_i \cdot \mathbf{w} \, dS \tag{5}$$

$$\langle \partial_t \eta \rangle = \partial_t(\varepsilon \langle \eta \rangle^i) - \frac{1}{V_0} \int_{\mathcal{A}_i} \mathbf{n}_i \cdot \mathbf{v}_i \, \eta \, dS \tag{6}$$

Where $\mathcal{A}_i$ is the interface surface between the void part and the no-void part of the REV, $\mathbf{n}_i$ is the normal to $\mathcal{A}_i$ with the sense from no-void part to void one.
Averaging unknown terms are produced. These terms are not fully defined by the average flux variables thus they must be set using a external theory. In this work, among unknown terms, the dispersion ones are taken in account.
In this work a compressible gas in laminar flow is considered. The gas is composed of oxygen(O_2) and nitrogen(N_2) and its temperature is constant. The gas fills fully the (connected)pores of the permable media.
To handle and solve equations is used COMSOL with its Equation-Based Modeling.

2 Governing Equations

The gas equation of state is

$$p = \rho\, R\, T \left(\frac{Y_1}{M_1} + \frac{1 - Y_1}{M_2} \right) \tag{7}$$

Where
p is the pressure,
R is the universal gas constant,
T is the absolute temperature,
Y_1 is the oxygen mass fraction,
M_1 is the oxygen molecular weight,
M_2 is the nitrogen molecular weight.
The mass balance of the flux in free space is expressed by

$$\partial_t \rho + \nabla \cdot (\rho\, \mathbf{v}) = 0 \tag{8}$$

$$\partial_t \rho_1 + \nabla \cdot (\rho\, Y_1\, \mathbf{v} - \rho\, D\, \nabla Y_1) = 0 \tag{9}$$

Where
ρ is the density,
$\mathbf{v}$ is the velocity,
ρ_1 is the oxygen density ($\rho_1 = Y_1\, \rho$),
D is the diffusion constant (oxygen-nitrogen).
The average of the equation 7 is

$$\begin{aligned} \langle p \rangle^i = \langle \rho \rangle^i\ R\, T \left(\tfrac{\langle Y_1 \rangle^i}{M_1} + \tfrac{1 - \langle Y_1 \rangle^i}{M_2} \right) + \\ + R\, T \left(\tfrac{\left\langle \rho^{\ominus}\, Y_1^{\ominus} \right\rangle^i}{M_1} - \tfrac{\left\langle \rho^{\ominus}\, Y_1^{\ominus} \right\rangle^i}{M_2} \right) \end{aligned}$$

Hereafter we take that

$$\rho^{\ominus} = 0 \tag{10}$$

It follows that

$$\langle p \rangle^i = \langle \rho \rangle^i\ R\, T \left(\frac{\langle Y_1 \rangle^i}{M_1} + \frac{1 - \langle Y_1 \rangle^i}{M_2} \right) \tag{11}$$

Using 5 and 6 the averaging of the equation 8 gives

$$\begin{aligned} \partial_t (\varepsilon \,\langle \rho \rangle^i) - \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i \cdot \mathbf{v}_i\, \rho\, dS + \\ + \nabla \cdot (\varepsilon \,\langle \rho\, \mathbf{v} \rangle^i) + \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i \cdot \rho\, \mathbf{v}\, dS = 0 \end{aligned}$$

The algebraic sum of the 2nd and the 4th term

$$\frac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i \cdot (\mathbf{v} - \mathbf{v}_i)\, \rho\, dS$$

is zero because

$$\mathbf{n}_i \cdot (\mathbf{v} - \mathbf{v}_i) = 0 \tag{12}$$

Indeed, the left side of 12 is the normal component of the relative velocity of the fluid on the solid, that must be zero (i.e. the fluid does not enter into the solid and does not separate from it). Using the property of the average operator we can write

$$\langle \rho\, \mathbf{v} \rangle^i = \langle \rho \rangle^i \,\langle \mathbf{v} \rangle^i + \left\langle \rho^{\ominus}\, \mathbf{v}^{\ominus} \right\rangle^i$$

The 2nd term of the right side is a dispersion term, but using 10 it is null. So the averaged mass balance, i.e. the mass balance of flux in permeable media, is expressed by

$$\partial_t (\varepsilon \,\langle \rho \rangle^i) + \nabla \cdot (\varepsilon \,\langle \rho \rangle^i \,\langle \mathbf{v} \rangle^i) = 0 \tag{13}$$

Using 5 and 6, defining

$$\mathbf{\Gamma}_1 = \rho\, Y_1\, \mathbf{v} - \rho\, D\, \nabla Y_1$$

the averaging of the equation 9 gives

$$\begin{aligned} \partial_t (\varepsilon \,\langle \rho_1 \rangle^i) - \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i \cdot \mathbf{v}_i\, \rho_1\, dS + \\ + \nabla \cdot (\varepsilon \,\langle \mathbf{\Gamma}_1 \rangle^i) + \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i \cdot \mathbf{\Gamma}_1\, dS = 0 \end{aligned}$$

The algebraic sum of the 2nd and the 4th term is

$$\frac{1}{V_0} \int\limits_{\mathcal{A}_i} (\mathbf{n}_i \cdot (\mathbf{v} - \mathbf{v}_i) \rho_1 - \mathbf{n}_i \cdot \rho\, D\, \nabla Y_1)\, dS$$

Due to 12 and taking the diffusion flux equal zero on the interface solid-fluid, it is zero. The averaged equation becomes

$$\partial_t (\varepsilon \,\langle \rho\, Y_1 \rangle^i) + \nabla \cdot (\varepsilon \,\langle \mathbf{\Gamma_1} \rangle^i) = 0 \tag{14}$$

Using the property of the average operator and 10 we can write

$$\begin{aligned} \langle \mathbf{\Gamma_1} \rangle^i \quad = \quad & \langle \rho \rangle^i \,\langle Y1 \rangle^i \,\langle \mathbf{v} \rangle^i + \langle \rho \rangle^i \left\langle Y_1^{\ominus} \mathbf{v}^{\ominus} \right\rangle^i + \\ & - D\ \langle \rho \rangle^i \,\langle \nabla Y_1 \rangle^i \end{aligned} \tag{15}$$

Using 4

$$\begin{aligned} \varepsilon \,\langle \nabla Y_1 \rangle^i = \nabla (\varepsilon \,\langle Y_1 \rangle^i) + \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i\, Y_1\, dS = \\ = \varepsilon \nabla \,\langle Y_1 \rangle^i + \tfrac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i\, (Y_1 - \langle Y_1 \rangle^i)\, dS \end{aligned} \tag{16}$$

The last equality is obtained by mean of

$$\nabla \varepsilon = - \frac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i\, dS \tag{17}$$

that is deduced from 4. The following equation is taken as arbitrary hypothesis.

$$\frac{1}{V_0} \int\limits_{\mathcal{A}_i} \mathbf{n}_i\, (Y_1 - \langle Y_1 \rangle^i)\, dS = 0 \tag{18}$$

The dispersion term is

$$\varepsilon \langle\rho\rangle^i \left\langle Y_1^{\ominus}\mathbf{v}^{\ominus}\right\rangle^i \quad (19)$$

It is modelled as follows

$$\left\langle Y_1^{\ominus}\mathbf{v}^{\ominus}\right\rangle^i = -\alpha \frac{1}{V_r} \langle\mathbf{v}\rangle^i \cdot \langle\mathbf{v}\rangle^i L_r \nabla \langle Y_1\rangle^i \quad (20)$$

Where α is an dimensionless parameter,
V_r is a reference velocity,
L_r is a length reference.
So the averaged oxygen mass fraction balance is expressed by

$$\begin{aligned}&\partial_t(\varepsilon \langle\rho\rangle^i \langle Y_1\rangle^i) + \nabla\cdot(\varepsilon \langle\rho\rangle^i \langle Y_1\rangle^i \langle\mathbf{v}\rangle^i + \\ &-\varepsilon \langle\rho\rangle^i \alpha \tfrac{1}{V_r} \langle\mathbf{v}\rangle^i \cdot \langle\mathbf{v}\rangle^i \, L_r \nabla \langle Y_1\rangle^i + \\ &-\varepsilon \langle\rho\rangle^i \, D \nabla \langle Y_1\rangle^i) = 0\end{aligned} \quad (21)$$

The following Ergun's model, as reported in [2], is used for momentum balance of flux in permeable media.

$$-\nabla \langle p\rangle^i = \mu \, \langle\mathbf{v}\rangle^i \frac{1}{K}(0.83 + 0.19 \, \hat{R}_{e_K}) \quad (22)$$

Where

$$\hat{R}_{e_K} = \frac{\rho \left|\langle\mathbf{v}\rangle^i\right|}{\mu}\sqrt{\frac{K}{\varepsilon}} \quad (23)$$

is the Reynolds number based on permeability,

$$K = \frac{d_p^2 \, \varepsilon^3}{36 \, k \, (1-\varepsilon)^2} \quad (24)$$

is the permeability computed by mean of the Kozeny-Carmans correlation [2].

3 Methods

To evaluate the effect of the dispersion term 19, it is simulated a blender (picture 1) with 2 inlet and 1 outlet. Through the inlet on the left side comes oxygen, through the other the nitrogen. The blender is filled with a granular media. The aim is to study the influence of the dispersion term on the course of $\langle Y_1\rangle^i$ along the blender. To do this α takes a succession of values. The model is 2D.

4 Numerical Model

The simulations are performed with the software COMSOL 4.2. The elements are triangular (picture 2) generated with a free mesh procedure with shape function linear and quadratic. All the simulations are static. Equation-Based Modelling is utilized. SI unit system is utilized. Except the inlets and the outlet, on all the boundaries there is the following constrain

$$\langle\mathbf{v}\rangle^i \cdot \mathbf{n} = 0 \quad (25)$$

The diffusion flux is zero on all boundaries except the inlets. The dispersion flux are zero on all boundaries except the inlets and the outlet. The pressure on the outlet is constrained to $1.0bar$, $\langle Y_1\rangle^i = 1$ on the O_2-inlet and $\langle Y_1\rangle^i = 0$ on the N_2-inlet. On the inlets is imposed an input mass flux equal to $0.001[m/s]\cdot 1.283[kg/m^3]$. The temperature is $T = 300K$.The porosity is $\varepsilon = 0.4$. The particle diameter is $d_p = 0.0001$. The tortuosity factor is $k = 5$. The D is considered constant.

5 Experimental Results

The results reported in the next pictures and graphs, are calculated for $\alpha = (0 : 5 : 50)$. In picture 3 is shown $\langle Y_1\rangle^i$ at $y = 0$, in picture 4 is shown $\langle Y_1\rangle^i$ at $y = 2.5$ (the outlet). In the pictures from 5 to 15 is shown a 2D surface plot of $\langle Y_1\rangle^i$ for the α succession.

6 Discussion

How it can be see from results, $\langle Y_1\rangle^i$ is strongly influenced by the parameter α. For example for $\alpha = 50$ at the end of the blender the gas has a quasi-uniform composition.

7 Conclusions

This study has demonstrated that the dispersion can be very important in the flux of a fluid in a permeable media. Furthermore it can suggest a method to verify experimentally the influence of dispersion and to determine α.

8 Figures

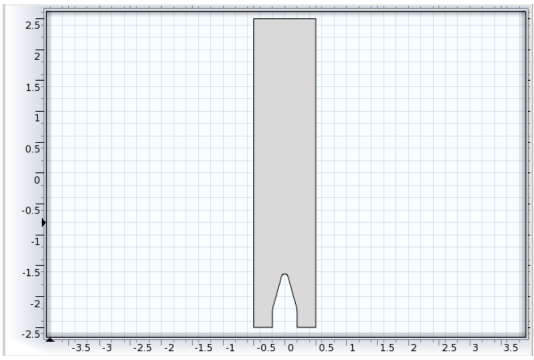

Figure 1: geometry

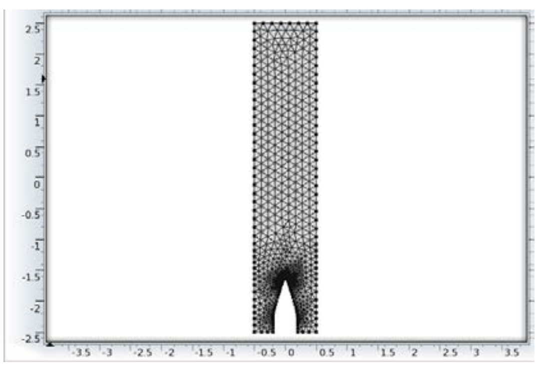

Figure 2: mesh

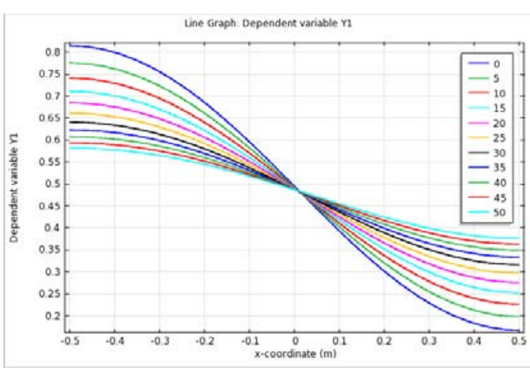

Figure 3: $\langle Y_1 \rangle^i$ at $y = 0$

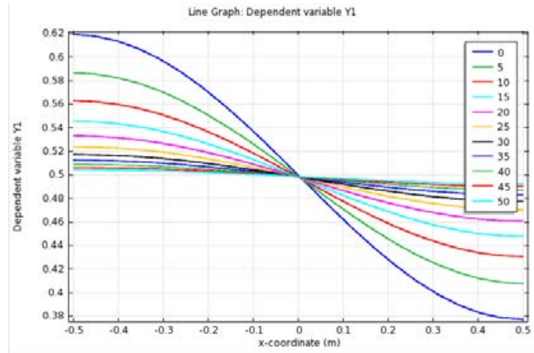

Figure 4: $\langle Y_1 \rangle^i$ at $y = 2.5$

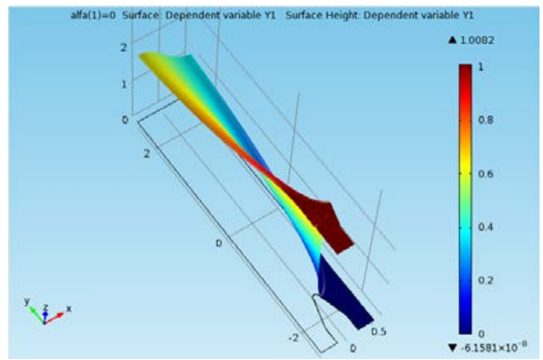

Figure 5: $\langle Y_1 \rangle^i$ for $\alpha = 00$

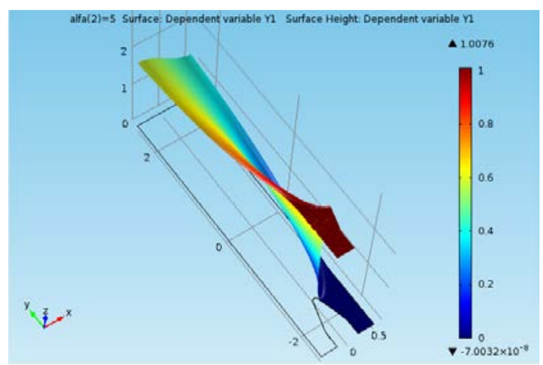

Figure 6: $\langle Y_1 \rangle^i$ for $\alpha = 05$

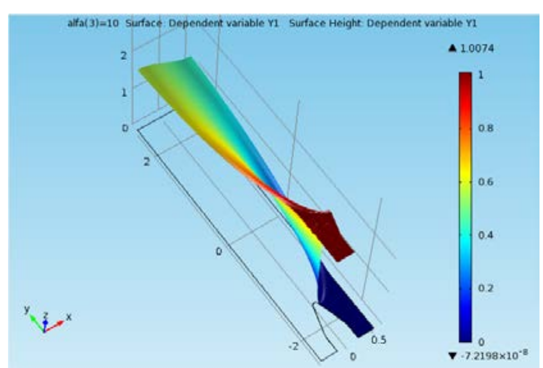

Figure 7: $\langle Y_1 \rangle^i$ for $\alpha = 10$

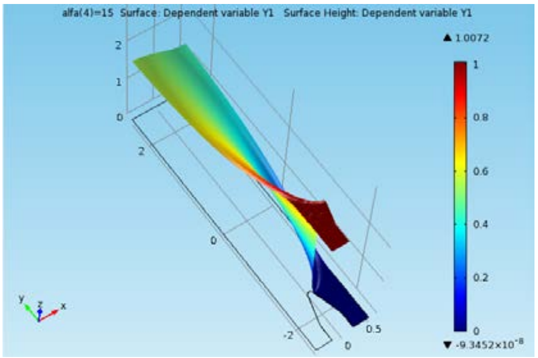

Figure 8: $\langle Y_1 \rangle^i$ for $\alpha = 15$

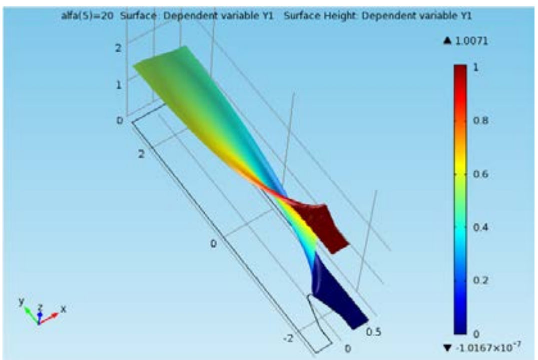

Figure 9: $\langle Y_1 \rangle^i$ for $\alpha = 20$

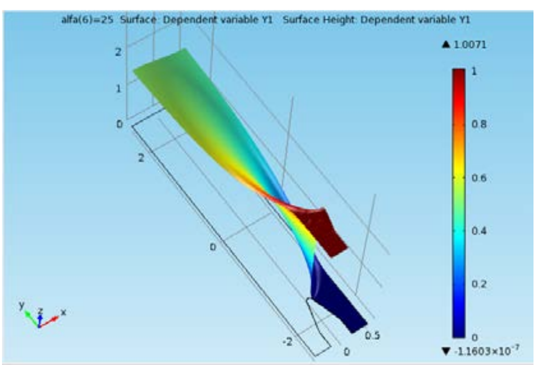

Figure 10: $\langle Y_1 \rangle^i$ for $\alpha = 25$

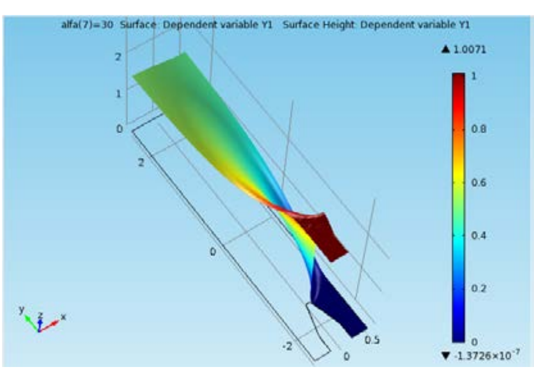

Figure 11: $\langle Y_1 \rangle^i$ for $\alpha = 30$

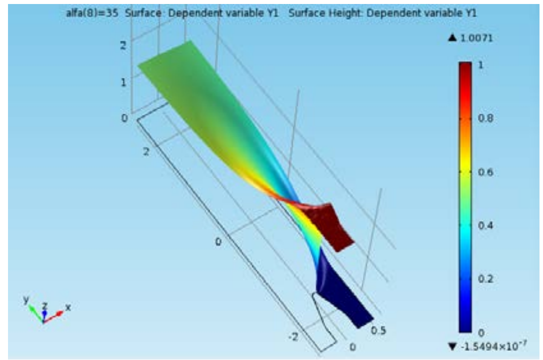

Figure 12: $\langle Y_1 \rangle^i$ for $\alpha = 35$

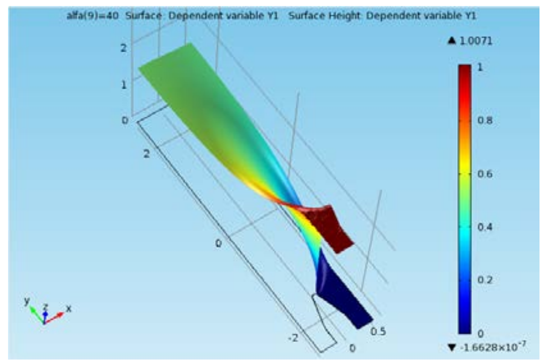

Figure 13: $\langle Y_1 \rangle^i$ for $\alpha = 40$

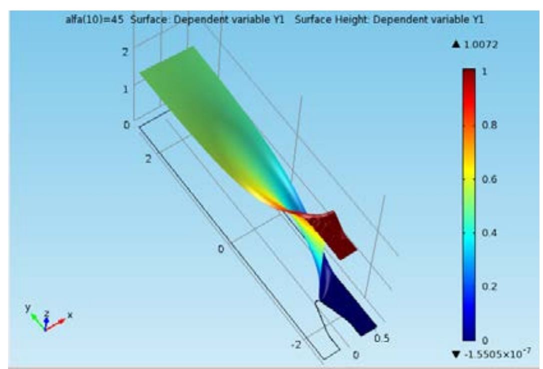

Figure 14: $\langle Y_1 \rangle^i$ for $\alpha = 45$

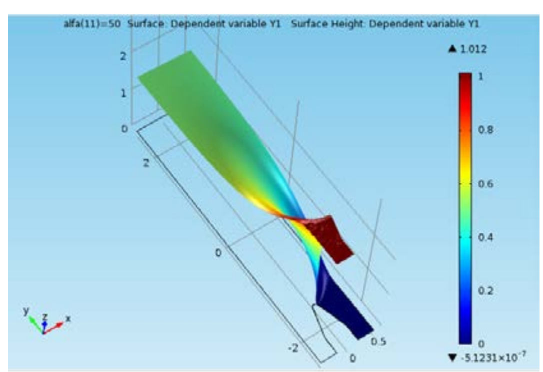

Figure 15: $\langle Y_1 \rangle^i$ for $\alpha = 50$

References

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[2] A. Jafari P. Zamankhan S.M. Mousavi K. Pietarinen, *Modeling and cfd simulation of flow behavior and dispersivity through randomly packed bed reactors*, Chemical Engineering Journal (2008).