STUDY OF ISOTHERMAL DIFFUSION IN POROUS MEDIA USING DIRECT NUMERICAL SIMULATION

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REZUMAT. Simularea numerică directă este o metodă de rezolvare a turbulenţelor care pot apărea la transferul de masă prin materiale poroase. În multe cazuri, simularea nu poate fi efectuată pentru întregul sistem, datorită dimensiunii discretizării. Oricum, difuzia este un proces care are loc la nivel microscopic şi, prin urmare, forţele de vâscozitate nu mai au nicio influenţă, iar concentraţia în fiecare punct al mediului poros nu are o semnificaţie practică. Astfel, sunt importante doar cantităţile fizice globale, precum fluxul de substanţă care traversează materialul în orice moment. Scopul acestei lucrări este de a face o comparaţie între fluxul de difuzie care traversează un material poros cu o geometrie cunoscută şi fluxul care trece prin acelaşi mediu, considerat omogen, având caracteristici globale cunoscute, în aceleaşi condiţii iniţiale şi de frontieră.

Cuvinte cheie: difuzie, vapori, materiale poroase, textile, simulare numerică, COMSOL Multiphysics®.

ABSTRACT. The direct numerical simulation is a method of solving the turbulences that can occur at mass transfer through porous media. In many cases the simulation cannot be performed for the entire system due to the meshing scale. However, the diffusion is a process that occurs at a microscopic level and therefore the viscosity forces have no longer any influence and the concentration at each point of the porous environment has not a practical significance. Thus, only the global physical quantities, such as the flow of substance that crosses the material at any time, are important. The goal of this study is to make a comparison between the diffusion flow that crosses a porous material with a known geometry and the flow passing through the same homogeneous medium having known global characteristics regardless the geometry of the system under the same initial and frontier conditions.

Keywords: diffusion, water vapor, porous media, textiles, numerical simulation, COMSOL Multiphysics®

1. INTRODUCTION

1.1. COMSOL Multiphysics® software

COMSOL Multiphysics® is a software that allows modeling and simulation of physical processes based on finite element theory [4]. There is the possibility to joint multiple physical processes that take place simultaneously and interact each with other, such as the heat and moisture transfer through porous media. The program has a large number of predefined interfaces (Fig. 1).

- Thermal transfer
- Fluids flow
- Chemical reactions and species transport
- Electricity and magnetism
- Mechanical stress of structures
- Acoustic etc.

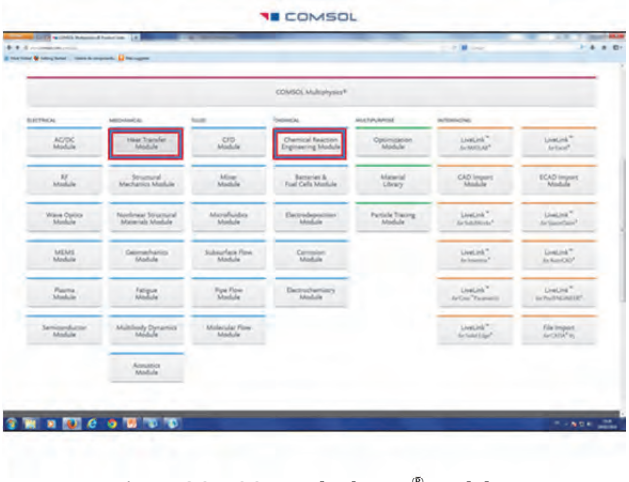

Fig. 1. COMSOL Multiphysics® modules.

Due to these interfaces and predefined models, simulation is much easier because the concern is mainly on defining relevant physical quantities such as material properties (ex. loads, constraints, sources

and flows) and it is not necessary to define the equations. For the same reason, there is no need in-depth knowledge of numerical analysis.

At the basis of the modeling are the partial differential equations (PEDs) that can be described in three forms [2]:

- Equations with coefficients, which define a linear pattern (or which can be considered linear);
- General equations (characteristic of nonlinear models);
- Weak Form Equations for PEDs that use mixed spaces and partial time derivatives.

The analysis of the studied phenomena can be done in several ways:

- Stationary analysis;
- Time-dependent analysis;
- User defined analysis (linear or nonlinear, eigenvalues of frequency etc.).

Although the COMSOL Multiphysics® software has weak tools of design (CAD only at a basic level), it is possible to import drawings from other environments such as CATIA, Inventor, SolidWorks or Pro/Engineer. COMSOL Multiphysics® software has also other modules that facilitate to create models and access to results. There is also the possibility to inquiry the COMSOL Multiphysics® program by other macroinstruction programming platforms (LiveLink ™ for MatLab, LiveLink ™ Excel etc.) [3].

1.2. COMSOL Multiphysics® graphic Interface

The user graphic interface of COMSOL Multiphysics® (GUI) is intuitive and multi-level structured application (Fig. 2), respecting the principle of inheritance from Object Oriented Programming [2, 4].

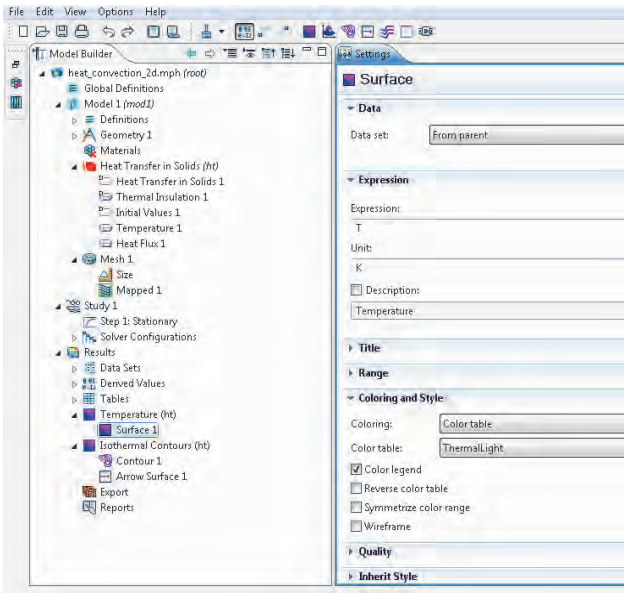

Fig. 2. Graphical user interface.

Building the model (Model Builder) is interactively, starting on the size of the workspace (3D, 2D, 1D, 0D), and then the physical phenomenon and the type of study (stationary, non-stationary etc.) can be chosen. The software builds itself a predefined model that can be updated by deleting or adding new nodes. For each model, the following structure is generated:

- Defining the variables and parameters;
- The geometric model;
- Physical phenomenon;
- Meshing mode;
- Type of analysis;
- Results.

2. ISOTHERMAL WATER VAPOR DIFFUSION IN POROUS MATERIAL

The goal of this study is to make a comparison between the diffusion flow that crosses a porous material with a known geometry and the flow passing through the same homogeneous medium having known global characteristics regardless the geometry of the system under the same initial and frontier conditions. Two different models of porous media are used. In the first model, a two-dimensional elementary domain from a porous medium (a 2D section) was taken into account, obtaining an effective value of diffusion and porosity. In the second model a one-dimensional simplification was used that have the effective diffusion coefficient from the first simulation.

2.1. Two-dimensional model

The geometric representation of the two-dimensional model is presented in Fig. 3. The vertical sides (L_0) represent the frontiers of mass transfer. The green colored area represents the void space for which the initial condition is the water vapor concentration c_0. The diffusion equation is given by Fick's law [7]:

$$\frac{\partial c}{\partial t} + \nabla \cdot \left(- D_a \cdot \nabla c\right) = 0 \qquad (1)$$

where c represents the molar concentration of water vapor in [mole/m^2] and D_a is the coefficient of water vapor diffusion in air, [m^2/s].

For the left border the limit condition is the concentration, $c_{\max}$, that have a fixed value. At the right border there is a mass transfer into the atmosphere by free convection, according to the following equation [8]:

$$\left(-D_a \cdot \nabla c\right) \cdot \vec{n} = h_m \cdot \left(c - c_\infty\right)\Big|_{x=L} \qquad (2)$$

where h_m is the mass transfer coefficient [m/s], c_∞ is the molar concentration of water vapor in the atmosphere at a sufficiently long distance from the border and $\vec{n}$ represents the normal direction vector on the border.

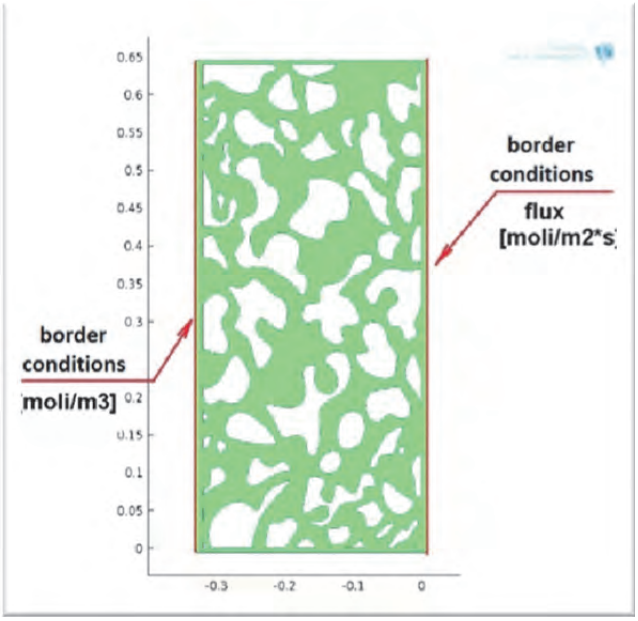

Fig. 3. 2D Porous Media

The average flow rate through this border is obtained using a mean function of the COMSOL.

In order to calculate the porosity, the two variables *V_gol* and *V_total* are defined as the integral of the elementary surfaces on the two domains. Porosity represents their ratio and is calculated automatically by the program according to Equation (3) [6]:

$$\varepsilon = \frac{V\_gol}{V\_total} \tag{3}$$

A time-dependent study was selected over the range {0; 0.1} [s]. At the moment t = 0.1 [s] the water vapor concentration in the system is shown in Fig. 4 and the diffusion flux magnitude in Fig.5.

To calculate effective diffusion, the Fick's first law was used, from where the following equation was obtained [1]:

$$D_{ef} = \phi \cdot \frac{L}{(c_{max} - c)} \tag{4}$$

where D_{ef} is the effective diffusivity in [m^2/s], ϕ represents the flow in [mole/m^{2}s], L is the thickness of the porous media in [m], and $(c_{max} - c)$ is the difference in concentration between the two boundaries of the system in [mole/m^2].

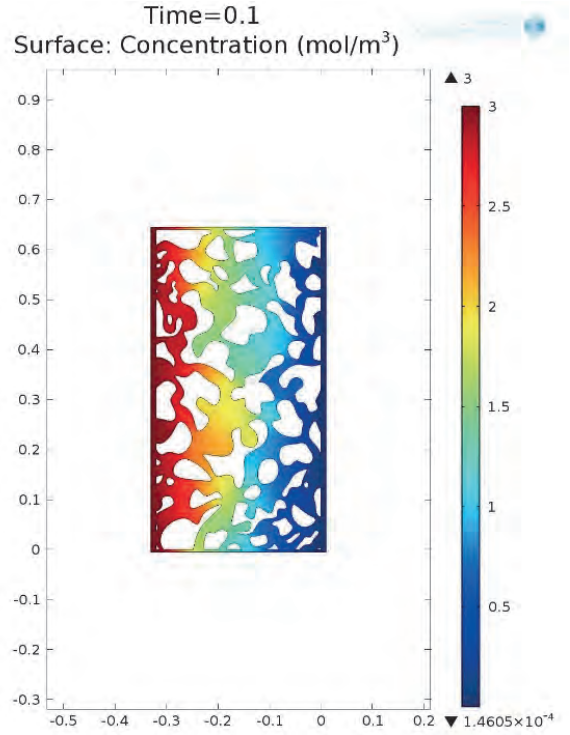

Fig. 4. Water vapor concentration, t = 0.1 s

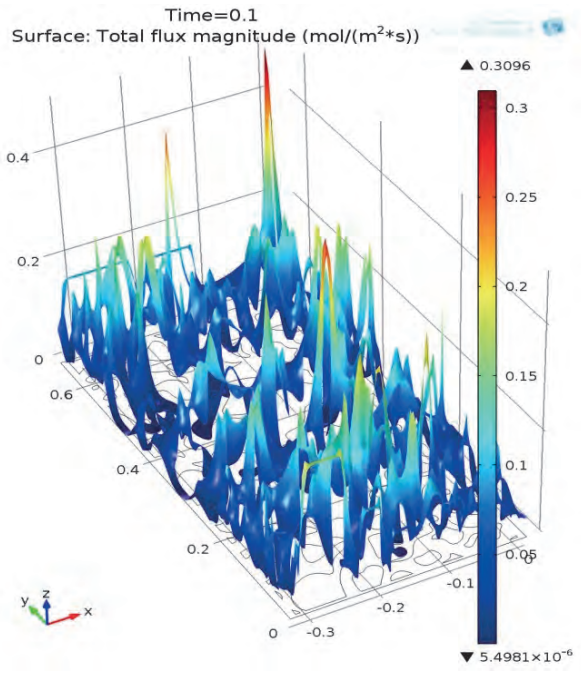

Fig. 5. The diffusion flux magnitude

The effective average diffusion that is calculated with the following integral on the border [5]:

$$D_{med} = \frac{1}{L_0} \int_0^{L_0} \phi(y) \cdot \frac{L}{(c_{max} - c(y))} \cdot dy \tag{5}$$

where $\phi(y)$, [mole/m^{2}s] represents the flow across the L_0 boundary that have the thickness L, $c(y)$ is the water vapor concentration at the border in [moles/m^2] and dy represents the mesh size.

2.2. One-dimensional model

For the second model a one-dimensional porous medium was considered, having the diffusion and porosity property determined above, and having the same size as the first model. The differential equation of diffusion becomes [2]:

$$\varepsilon \cdot \frac{\partial c}{\partial t} + \nabla \left(- D_{efectiv} \nabla c \right) = 0 \qquad (6)$$

The average diffusion coefficient obtained (4.12 $*10^{-6}$ m^2/s) and the porosity (0.6415) are introduced in the one-dimensional model as the properties of porous media.

2.3. Comparison between the models

The graphical representation of the average flow for the two simulations is shown in Fig.6.

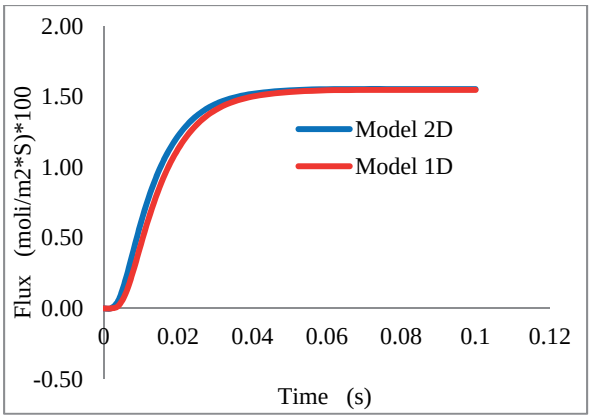

Fig. 6. Molar flow of water vapors

As shown in Fig. 6, the fluxes for both one-dimensional and two-dimensional models have a similar evolution. The one-dimensional model being simpler does not have the problems of mesh, whereas the two-dimensional model requires a very fine meshing structure.

If the geometric dimensions of the 2D model are greatly increased, this form of meshing becomes expensive or even impossible.

3. CONCLUSION

Modeling (from diffusion point of view) the porous media which can be considered homogeneous can be simplified taking into account only global parameters such as porosity or effective diffusion coefficient. Global parameters can be measured experimentally by different methods, or they can result from a simulation on a much more restrained field such as the two-dimensional one.

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