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## Молекулярно-динамическое моделирование процессов взаимодействия водяного пара с несквозными порами цилиндрического типа

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Теоретические и экспериментальные исследования взаимодействия водяного пара с пористыми материалами проводятся как на макро-, так и на микроуровне. На макроуровне исследуется влияние структуры расположения индивидуальных пор на процессы взаимодействия водяного пара с пористым материалом как сплошной средой. На микроуровне исследуется зависимость характеристик взаимодействия водяного пара с пористой средой от геометрии и размеров индивидуальной поры.

В данной работе проведено исследование посредством математического моделирования процессов взаимодействия водяного пара с индивидуальной несквозной порой цилиндрического типа. Вычисления производились с использованием модели гибридного типа, сочетающей в себе молекулярно-динамический и макродиффузионный подходы для описания взаимодействия водяного пара с индивидуальной порой. Исследовались процессы эволюции к состоянию термодинамического равновесия макроскопических характеристик системы, таких как температура, плотность, давление, в зависимости от внешних по отношению к поре условий. Проведено исследование зависимости параметров эволюции от распределения значений коэффициента диффузии в поре, полученного в результате молекулярно-динамического моделирования. Актуальность данных исследований обусловлена тем, что все используемые для моделирования влаго- и теплопроводности методы и программы основаны на применении уравнений переноса в пористом материале (как сплошной среде) с известными заранее значениями коэффициентов переноса, которые, как правило, получены экспериментально.

Ключевые слова: пористые среды, молекулярная динамика, макроскопическая диффузионная модель

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## Molecular-dynamic simulation of water vapor interaction with suffering pores of the cylindrical type

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Theoretical and experimental investigations of water vapor interaction with porous materials are carried out both at the macro level and at the micro level. At the macro level, the influence of the arrangement structure of individual pores on the processes of water vapor interaction with porous material as a continuous medium is studied. At the micro level, it is very interesting to investigate the dependence of the characteristics of the water vapor interaction with porous media on the geometry and dimensions of the individual pore.

In this paper, a study was carried out by means of mathematical modelling of the processes of water vapor interaction with suffering pore of the cylindrical type. The calculations were performed using a model of a hybrid type combining a molecular-dynamic and a macro-diffusion approach for describing water vapor interaction with an individual pore. The processes of evolution to the state of thermodynamic equilibrium of macroscopic characteristics of the system such as temperature, density, and pressure, depending on external conditions with respect to pore, were explored. The dependence of the evolution parameters on the distribution of the diffusion coefficient in the pore, obtained as a result of molecular dynamics modelling, is examined. The relevance of these studies is due to the fact that all methods and programs used for the modelling of the moisture and heat conductivity are based on the use of transport equations in a porous material as a continuous medium with known values of the transport coefficients, which are usually obtained experimentally.

**Keywords:** porous media, molecular dynamics, macroscopic diffusion model

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## Introduction

One of the most important problem for theoretical and experimental investigations of water vapor interaction with porous materials is how to combine calculation results obtained by micro level study, for example molecular dynamic and Monte-Carlo simulation, analytical investigations by solving mass transfer equations for single pore etc. [Alim et al., 2017] with experimental data and calculations by empirical formulas which is usually presented by macro characteristics such as porosity, density etc. [Krus, 1996]. At the macro level, the influence of the arrangement structure of individual pores on the processes of water vapor interaction with porous material as continuous medium is ordinary studied. But even at the level of individual pore molecular dynamic simulation data does not directly correspond to macro characteristics of water vapor interaction with a pore. So if macro equations like, for example, diffusion equations can be solved for some geometry of the pore it would be useful to use the following two steps solution scheme. At the first step we can obtain some characteristics like, for example, diffusion coefficient by molecular dynamic simulations. At the second step we can use the values of these diffusion coefficients for solving diffusion equations at the macro level. Moreover, the dependence of the characteristics of the water vapor interaction with porous media on the geometry and dimensions of the individual pore can be investigated at the micro level, in more simple way then in the case of diffusion or mass transfer equations, at macro level.

In this paper, processes of water vapor interaction with suffering pore of the cylindrical type are considered. Investigations are carried out by means of mathematical modelling. The calculations are performed using hybrid model combining molecular dynamic and a macro-diffusion approach for describing water vapor interaction with individual pore, like in [Nikonov et al., 2017a; Nikonov et al., 2017b]. The processes of evolution to the state of thermodynamic equilibrium of macroscopic characteristics of the system such as temperature, density, and pressure, depending on external conditions with respect to pore, is explored. The dependence of the evolution parameters on the distribution of the diffusion coefficient in the pore, obtained as a result of molecular dynamics modelling, is researched. The topicality of these explorations is due to the fact that all methods and programs used for the modelling of the heat and moisture conductivity are based on the use of transport equations in porous material as continuous medium with known values of transport coefficients. These coefficients are usually obtained experimentally or using empirical formulas. Analysis of the following modern software for Modelling of Heat, Air, Moisture (HAM) transfer through porous media is carried out.

- The Heat, Air and Moisture Tool Kit (Quirouette Building Science Software, <http://www.qbstoolbox.com/>).
- NRC-IRC hygIRC-1-D: helps design community choose optimal building envelope components and systems (<https://www.nrc-cnrc.gc.ca/eng/projects/irc/hygirc.html>).
- WUFI - Oak Ridge National Laboratory (ORNL)/Fraunhofer IBP is a menu-driven PC program which allows realistic calculation of the transient coupled one-dimensional heat and moisture transport in multi-layer building components exposed to natural weather. It is based on the newest findings regarding vapor diffusion and liquid transport in building materials and has been validated by detailed comparison with measurements obtained in the laboratory and on outdoor testing fields.
- COMSOL (<https://www.comsol.com>) for Modeling Heat and Moisture Transport in Building Materials is also very powerful and multifunctional software.

All of these programs use calculation methods for modelling of moisture transfer through porous media based on transport differential equations with previously known transport coefficients. So it is necessary to know values of the transport coefficients before using of these programs. One of the alternative ways

with respect to the experience is to obtain these coefficients by molecular dynamic simulations. We present this alternative in this paper.

## Molecular dynamics model

In classical molecular dynamics, the behavior of an individual particle is described by the Newton equations of motion [Gould et al., 2005], which can be written in the following form

$$m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{f}_i, \quad (1)$$

where  $i$  – a particle number ( $1 \leq i \leq N$ ),  $N$  – the total number of particles,  $m_i$  – particle mass,  $\vec{r}_i$  – coordinates of position,  $\vec{f}_i$  – the resultant of all forces acting on the particle. This resultant force has the following representation

$$\vec{f}_i = -\frac{\partial U(\vec{r}_1, \dots, \vec{r}_N)}{\partial \vec{r}_i} + \vec{f}_i^{ex}, \quad (2)$$

where  $U$  – the potential of particle interaction,  $\vec{f}_i^{ex}$  – a force caused by external fields. For a simulation of particle interaction, we use the Lennard-Jones potential [Lennard-Jones, 1924] with  $\sigma = 3.17 \text{ \AA}$  and  $\varepsilon = 6.74 \cdot 10^{-3} \text{ eV}$ . It is the most used to describe the evolution of water in liquid and saturated vapor form. The interaction between particles and the walls of the pore is described by one of the well-known potential (3) so called Lennard-Jones 9-3 wall potential [Siderius, Gelb, 2011].

$$U_{9-3}(r_{pw}) = 2\pi\alpha \left[ \frac{2}{45} \left( \frac{\sigma_{pw}}{r_{pw}} \right)^9 - \frac{1}{3} \left( \frac{\sigma_{pw}}{r_{pw}} \right)^3 \right]. \quad (3)$$

Here  $\alpha = \rho_w \sigma_{pw}^3 \varepsilon_{pw}$ ,  $\sigma_{pw}$  and  $\varepsilon_{pw}$  are the Lennard-Jones length and energy parameters for the interaction of a water molecule with a single constituent particle of the solid, and  $r_{pw}$  is the distance between the water molecule and the surface.  $\rho_w$  is the volume density of the surface material. In accordance with the paper [Das, Singh, 2013] it used for strongly attractive pore walls the following values  $\alpha = 4.27$  and  $\sigma_{pw} = 0.9462$  in molecular dynamic simulations. Equations of motion (1) were integrated by Velocity Verlet method [Verlet, 1967]. Nose–Hoover thermostat is used for temperature calibration and control. This method was originally introduced by Nose [Nosé, 1984] and subsequently developed by Hoover [Hoover, 1985]. The idea is to consider the heat bath as an integral part of the system by addition of an artificial variable  $\tilde{s}$ , associated with a “mass”  $Q > 0$  as well as a velocity  $\tilde{\dot{s}}$ . The magnitude of  $Q$  determines the coupling between the reservoir and the real system and so influences the temperature fluctuations. The artificial variable  $\tilde{s}$  plays the role of a time-scaling parameter, more precisely, the timescale in the extended system is stretched by the factor  $\tilde{s}$ :

$$d\tilde{t} = \tilde{s} dt.$$

## Molecular dynamic model calibration

It is used experimental data for the investigation of the time and space dependent moisture distribution in a drying brick sample [Pleinert et al., 1998] to adjust the values of the parameters  $Q$  and  $\tilde{s}$  of Nose–Hoover thermostat. The sample dimensions are  $12 \times 9 \times 3 \text{ cm}^3$ . All faces of the brick except for one face are isolated from the surrounding space by means of aluminum foil. Therefore evaporation can occur only through one open face along the length  $9 \text{ cm}$ . The open face is  $12 \times 3 \text{ cm}^2$ . Similarly to work [Amirkhanov et al., 2008], we take values of water concentration in points  $x = 89.1, 88.2, 87.3, 86.4, 85.5 \text{ mm}$  from the side of the open edge of the brick using the humidity distribution plot [Pleinert et al., 1998]. We get the following plot for these points at the left picture and corresponding approximation by the function  $w = a + be^{-t}$  at the right picture (Fig. 1). The values of the density

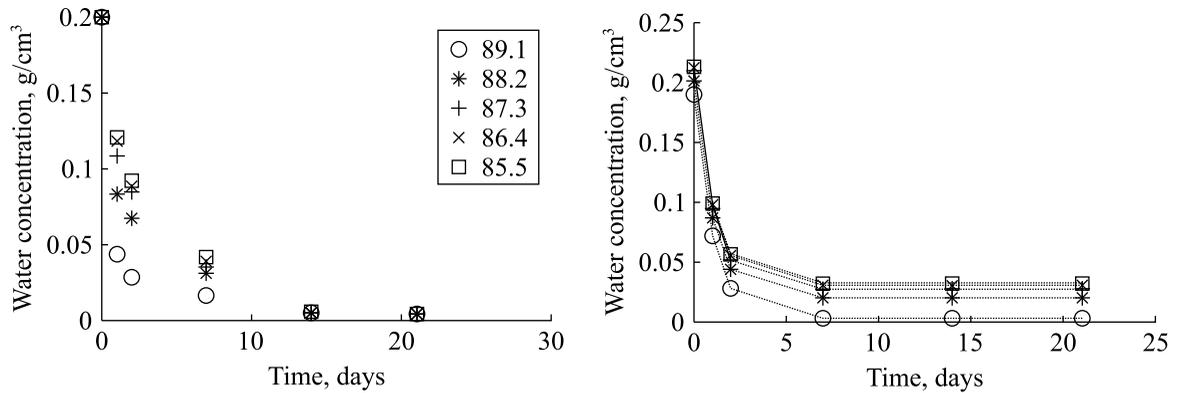


Figure 1. Dynamics of water concentration at boundary. The left figure shows the experimental values of water vapor concentration at points  $x = 89.1, 88.2, 87.3, 86.4, 85.5$  mm located near the open edge of the brick. The right figure shows the result of approximation of these points  $x = 89.1, 88.2, 87.3, 86.4, 85.5$  mm using the function  $w = a + be^{-t}$

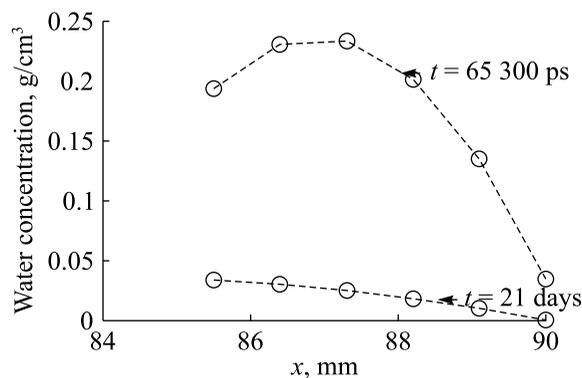


Figure 2. This figure shows the points that are the result of the time extrapolation of the data from Figure 1 using the  $w = a + be^{-t}$  function. The points for two moments of time  $t = 65\,300$  ps and  $t = 21$  days are presented. This figure also shows the result of the approximation of the water vapor concentration along the  $x$  coordinate for two moments of time  $t = 65\,300$  ps and  $t = 21$  days using the function  $w = ax^2 + bx + c$

of water vapor at points with coordinates  $x = 90, 89.1, 88.2, 87.3, 86.4, 85.5$  mm for the time point  $t_0 = 65\,300$  ps can be obtained by extrapolation in time using this function  $w = a + be^{-t}$ . These values of water vapor density for two time points  $t = 65\,300$  ps and  $t = 21$  days are shown in Figure 2 as circles. Consider the distribution of moisture at the boundary of the open edge at the point  $x = 90\text{ mm} - 250\text{ nm} = 89.999750\text{ mm}$ , for two times  $t = 65\,300$  ps and  $t = 21$  days. Here,  $t = 21$  days is an experimental time and  $t = t_0, t_0 = 65\,300$  ps is our simulation time. Approximation by the parabola  $w = ax^2 + bx + c$  leads to distributions of water concentration shown in figure 2 for these two time moments. Note, that  $x = 250\text{ nm}$  presents the middle of the pores which will be considered later. The value of the density of water vapor in the center of the pore at the point  $x = 89.999750\text{ mm}$  can be found by interpolation using the function  $w = ax^2 + bx + c$ . This is the value to which the density of water vapor should be equal at the time point  $t_0 = 65\,300$  ps, if there was 100% saturated water vapor in the pore at the time moment  $t = 0$ . Thus, we get the following values for water concentration in the  $x = 89.999750\text{ mm}$  layer. For  $t = 21$  days –  $w = 0.00041511\text{ g/cm}^3$  and for  $t = t_0$  –  $w = 0.034386\text{ g/cm}^3$ . The last value for water concentration is used for calibration of  $Q$  and  $\bar{s}$  parameters for the thermostat. The parameters of the Nose–Hoover thermostat  $Q$  and  $\bar{s}$  are selected so that at the end of the evolution, for the time moment  $t_0 = 65\,300$  ps, the system reaches a state in which the density of the water vapor in the pore would be equal  $w = 0.034386\text{ g/cm}^3$ . We use the ratio of water

concentration at time  $t = 0$  and  $t = t_0$  i.e.  $K = 0.2/0.034386 = 5.816321$  to calculate the number of water vapor molecules in the pore.

## Macroscopic diffusion model

Let us denote the water vapor concentration as  $w_v(r, \varphi, z, t)$  [ng/(nm)<sup>3</sup>] in the point  $(r, \varphi, z, t)$  where  $r, \varphi, z$  are space independent cylindrical variables and  $t$  is time independent variable. Then, we consider the following macroscopic diffusion model:

$$\frac{\partial w_v}{\partial t} = D \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial w_v}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 w_v}{\partial \varphi^2} + \frac{\partial^2 w_v}{\partial z^2} \right], \quad 0 < r < r_0, \quad 0 < \varphi < 2\pi, \quad 0 < z < z_0, \quad t > 0, \quad (4)$$

$$w_v(r, \varphi, z, 0) = w_{v,0}, \quad 0 \leq r \leq r_0, \quad 0 \leq \varphi < 2\pi, \quad 0 \leq z \leq z_0, \quad (5)$$

$$\frac{\partial w_v}{\partial r}(r_0, \varphi, z, t) = 0, \quad 0 \leq \varphi < 2\pi, \quad 0 \leq z < z_0, \quad t > 0, \quad (6)$$

$$\frac{\partial w_v}{\partial z}(r, \varphi, 0, t) = 0, \quad 0 \leq r < r_0, \quad 0 \leq \varphi < 2\pi, \quad t > 0, \quad (7)$$

$$-D \frac{\partial w_v}{\partial z}(r, \varphi, z_0, t) = \beta [w_v(r, \varphi, z_0, t) - w_{v,out}(t)], \quad 0 \leq r < r_0, \quad 0 \leq \varphi < 2\pi, \quad t > 0, \quad (8)$$

where  $D$  is the diffusion coefficient [(nm)<sup>2</sup>/psec];  $r_0, 2\pi, z_0$  are 3D pore cylindrical dimensions [nm];  $w_{v,0}$  is the initial concentration of water vapor;  $\beta$  is the coefficient of water vapor transfer from pore space to outer space [nm/psec];  $w_{v,out}(t)$  is the water vapor concentration in outer space [ng/(nm)<sup>3</sup>].

Because the initial (5) and boundary (6)–(8) conditions do not depend on the variable  $\varphi$ , the solution of the problem (4)–(8) does not depend on  $\varphi$ , so that  $w_v = w_v(r, z, t)$ .

We suppose that the outer space water vapor concentration is expressed as

$$w_{v,out}(t) = \varphi_0 \cdot w_{sv}(T_0),$$

where  $\varphi_0$  is the relative humidity of outer space ( $0 \leq \varphi_0 \leq 1$ ) and  $w_{sv}(T_0)$  is saturated water vapor concentration at outer temperature  $T_0$ .

In this case, the linear problem (4)–(8) can be solved exactly by means of the variables separation method [Bitsadze, Kalinichenko, 1980] and the result of the solution is the following:

$$w_v(r, z, t) = w_{sv}(T_0) \cdot \varphi_0 + [w_{v,0} - w_{sv}(T_0) \cdot \varphi_0] \sum_{m=1}^{\infty} \sum_{n=0}^{\infty} e^{D\lambda_{mn}t} c_{mn} J_0(\alpha_{rn}r) \cos(\alpha_{zm}z), \quad (9)$$

$$0 \leq r \leq r_0, \quad 0 \leq z \leq z_0, \quad t \geq 0.$$

Here,  $c_{mn}$  are coefficients of unity expansion

$$c_{mn} = \begin{cases} \frac{4 \sin(\alpha_{zm}z_0)}{2z_0\alpha_{zm} + \sin(2\alpha_{zm}z_0)}, & \text{if } n = 0, \quad m = 1, 2, 3, \dots, \\ 0, & \text{if } n = 1, 2, 3, \dots, \quad m = 1, 2, 3, \dots, \end{cases}$$

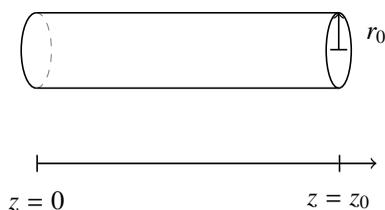


Figure 3. Shape of 3D pore

and  $\lambda_{mn}$  are eigenvalues where

$$\lambda_{mn} = -\alpha_{zm}^2 - \alpha_{rn}^2,$$

and  $\alpha_{zm}, \alpha_{rn}$  are solutions of the equations:

$$\begin{aligned} \alpha_{zm} \cdot \tan(\alpha_{zm}z_0) &= \beta/D, & m = 1, 2, 3, \dots, \\ J'_0(\alpha_{rn}r_0) &= 0, & n = 0, 1, 2, \dots, \end{aligned}$$

with  $J_0(x)$  as the Bessel function of the first kind of zero order.

## Computer simulations

Our micro model is made up of a pores in the shape of a cylinder with the radius  $r_0 = 28.5$  nm and the length  $z_0 = 500$  nm, the outer environment is simulated by a prism that is also 500 nm long and its sides are 150 nm, that is, the outer volume is 9 times greater than the cylinder volume.

Initial concentrations were obtained from the density of water vapor at the appropriate pressure and density at a given temperature using known tabulated data. The pressure in the pore was controlled using the well-known formula based on virial equation [Frenkel, Smith, 2002].

At a temperature  $T_0 = 25$  °C and pressure  $p_0 = 3.17$  kPa, 1000 molecules of water vapor are placed in the pore and 1800 molecules in the outer environment. The molecules are evenly distributed both in the pore and in the external environment. This means, we have 100 % saturated water vapor at a pressure  $p_0$  in the pore and 20 % of saturated water vapor in the outside. At the beginning moment  $t = 0$ , we give the particles random velocities from the interval  $(-1, 1)$  and set the total velocity equal to zero. Then, the velocities are re-scaled so that the desired initial kinetic energy is achieved for both the pore and the outside.

Under these conditions at time  $t = t_0$ , we expected  $N = 338$  molecules of water vapor in the pore resulting from the equation  $\frac{1000 - 200}{N - 200} = K$  where 200 molecules represent an outer concentration in our model.

To achieve the desired value at  $t = t_0$ , we use the following values  $Q = 14$  and  $\bar{s}(0) = 0.5$  for the Nose–Hoover thermostat. As a result at the time  $t = t_0$ , we have 338 particles in our model.

The main characteristic of the diffusion process is the diffusion coefficient. One goal of the micro model is to calculate a diffusion coefficient  $D$  which will then be used in the macro-model. Molecular dynamic simulations allow to get diffusion coefficients inside the pore  $D_{in}$  and out of the pore  $D_{out}$  by the well-known formula [Frenkel, Smith, 2002]. After averaging over time and volume the following values for diffusion coefficients  $D_{in} = 4.86$ ,  $D_{out} = 18.9$  are calculated and average for the pore and outer space value  $D_{avr} = 11.88$  nm<sup>2</sup>/ps.

For understanding of the differences between the traditional macro-description based on diffusion equation (4) with corresponding initial (5) and boundary conditions (6)–(8) and micro-description based on the molecular dynamic modeling it is compared the space mean value

$$w(t) = \frac{1}{\pi r_0^2 z_0} \int_0^{r_0} \int_0^{2\pi} \int_0^{z_0} w_v(r \cos \varphi, r \sin \varphi, z, t) r dr d\varphi dz$$

of water vapor concentration (WVC) obtained by solving of the diffusion equation with the WVC obtained by molecular dynamic simulations. The results are in the Fig. 4.

The graph in Figure 4 allows the following conclusions. Curves II, II, IV, obtained as a result of analytic calculations using formula (9), cannot describe with absolute accuracy the evaporation process in a blind pore due to the time dependence of the diffusion coefficient and the concentration of water

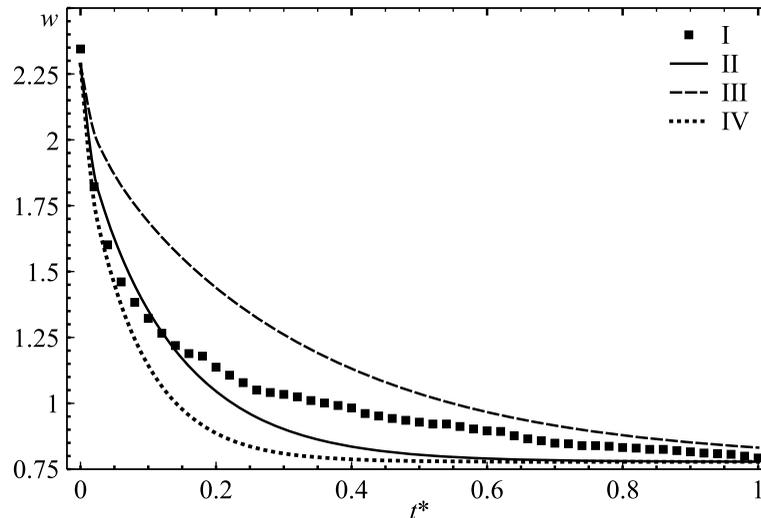


Figure 4. The dynamics of WVC obtained by diffusion equation and by molecular dynamics. Here a curve denoted as **I** is the result of molecular dynamic simulations, **II**, **III** and **IV** curves are analytic solutions of diffusion equation (4) for  $D_{avg} = 11.88$ ,  $D_{in} = 4.86$  and  $D_{out} = 18.9$   $\text{nm}^2/\text{ps}$  correspondingly. Units of  $w$  are [ $10^{-17}$   $\text{ng}/\text{nm}^3$ ]. Reduced time  $t^* = t/65320$  ps where  $t$  is measured in ps

vapor in the pore. This fact is confirmed by measurement data in experiments on the drying of the surface layer in homogeneous porous materials [Bianchi Janetti, 2018].

As far as can be judged from Figure 4, the calculated curve with a constant diffusion coefficient equal to the time and pore volume averaged inside the pore does not allow us to describe the behavior of the curve obtained as a result of molecular dynamic simulation (MD-curve) with an acceptable degree of accuracy. The curves obtained analytically with constant diffusion coefficients  $D_{in}$  and  $D_{out}$ , calculated inside and outside the pore, are rather far from a quantitative description of the MD-curve. Although the curve obtained with the diffusion coefficient  $D_{out}$ , satisfactorily describes the drying process up to the point in time  $t^* = 0.05$  in relative units. A more acceptable way of describing the drying process in a pore is the analytical curve calculated with a constant diffusion coefficient equal to the average between  $D_{in}$  and  $D_{out}$ . In this case, the nonlinearity of the diffusion coefficient of time and of the concentration of water vapor in the pore manifests itself, which is also confirmed experimentally [Bianchi Janetti, 2018].

A sharp drop in the MD curve up to the point in time  $t^* = 0.18$  in relative units indicates that the diffusion coefficient rises rather slowly during the time interval [0.0.18], remaining at the same time less in absolute value  $D_{avg}$ . This fact is explained by intensive evaporation, despite the fact that the density of water vapor in the pore remains quite high. From the moment of time  $t^* = 0.18$ , the MD-curve becomes flatter and passes above the theoretical curve for a constant diffusion coefficient  $D_{avg}$ . This means that the value of the diffusion coefficient is higher than the value of  $D_{avg}$  and grows more intensively than the diffusion coefficient in the time interval [0.0.18]. This fact is explained by the slowing down of the evaporation of water vapor from the pore due to a decrease in the total number of water molecules in the pore and an increase in the number of particles that interact with the pore walls. At the same time, the influx of new water molecules into the pore volume is lacking.

## Conclusions

Our investigations allow to affirm that an approach based on combination of diffusion coefficients determination by means of molecular dynamics and further application of these coefficients in macro model computations is useful for accuracy increasing of water-pore interaction description

if the most accurate diffusion coefficient map is used. In this case the simulation of moisture transfer through porous media by widely used in material science software such as WUFI, COMSOL etc. has to be more accurate without loss of calculation efficiency.

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