

Numerical Investigation of the Water Vapour Diffusivity inside Homogeneous Porous Media

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Abstract. This work is devoted to numerical investigation of diffusivity function for water vapour interaction with homogeneous porous media. Molecular dynamics simulation is used to determine the diffusivity function. Various approximations of diffusivity are applied for numerical solution of diffusion equation.

1 Statement of the problem

The investigation of the isothermal moisture absorption in unsaturated media is of fundamental interest in areas such as the issue of general safety rules, the physics of the buildings, the reactive transport of fluids through the Earth crust, etc. As a consequence, the study and modeling of the moisture transfer processes in porous materials is of permanent concern.

If the gravity is negligible in comparison with the capillary forces, then the isothermal absorption of the moisture (i.e., water vapour phase) in a macroscopically homogeneous porous material is governed by the one-dimensional diffusion equation [1],

$$\frac{\partial w(x, t)}{\partial t} = \frac{\partial}{\partial x} \left(D(w) \frac{\partial w(x, t)}{\partial x} \right), \quad (1)$$

where $w(x, t)$ denotes the local volumetric water content (m^3/m^3) and $D(w)$ the diffusivity (m^2/s).

Eq. (1) is solved with the initial and boundary conditions

$$w(t, 0) = w_1, \quad w(t, l_x) = w_2, \quad w(0, x) = \frac{w_2 - w_1}{l_x} \cdot x + w_1. \quad (2)$$

The equations (2) are written under the assumption that the behavior of the water vapour in a homogeneous porous medium is similar to the behavior of the water vapour in an individual through-type pore with suitable hydraulic properties [2–4].

In calculations $w_1 = 7.92 \text{ ng}/\text{nm}^3$ and $w_2 = 39.92 \text{ ng}/\text{nm}^3$ – the water vapour densities on the left end of the pore ($x = 0$) and on the right end of the pore ($x = l_x$) – has been used Eq. (2).

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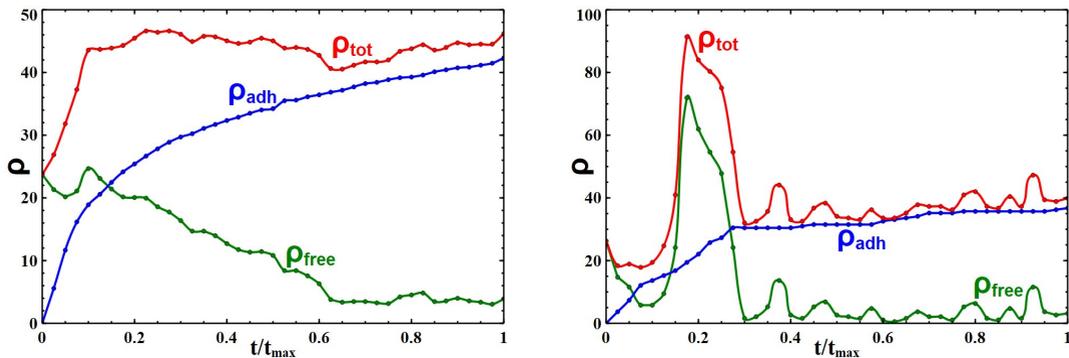


Figure 2. Time dependence of the densities averaged over the pore volume (left) and densities averaged over two central layers of the inner space of the pore (right). ρ is the density of the water vapour in $[\text{ng}/\text{nm}^3 \times 10^{-18}]$, $t_{\text{max}} = 16663.2$ ps.

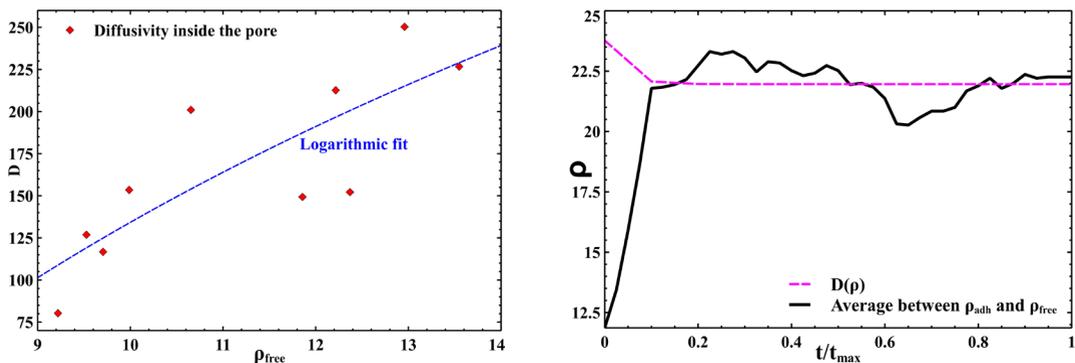


Figure 3. Approximation of the diffusivity as a function of ρ by the logarithmic function (left). Comparison of the averaged density-curves calculated by the diffusion equation with the logarithmic approximation of the diffusivity and MD-curves (right). ρ is the density of the water vapour in $[\text{ng}/\text{nm}^3 \times 10^{-18}]$, $t_{\text{max}} = 16663.2$ ps.

3 Computer simulations

Figure 2 presents the calculated time evolution for the density of adhered water molecules ρ_{adh} , the density of moving water molecules ρ_{free} and the total density of the water molecules in the pore ρ_{tot} averaged over the pore (left picture) and at the center of the pore (right picture).

Figure 3 left presents the logarithmic approximation of the diffusivity function. This approximation is used for the numerical solution of the diffusion equation (1) by an implicit finite difference scheme [12]. Results of the diffusion equation solution (1) are presented in Figure 3 right.

As can be seen from Figure 3 right, the logarithmic approximation of the diffusivity function in concentration ρ make it possible to better describe the time evolution of the concentration of the water vapour averaged over the molecules moving in, respectively adhering to the pore.

4 Conclusions

Our simulations show that the water vapour interaction with a porous media the diffusivity presents a very complicated dependence on the density. Molecular dynamics simulations produce a sufficiently realistic picture of the water vapour interaction with a pore if the computer model takes into account the interaction of the water molecules with the pore walls. The solution of the diffusion equation strongly depends on the average between the density of stuck liquid water molecules and the density of moving liquid water molecules but not on the total density of water vapour as a function of time and coordinates.

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