Resolving of Inverse Problem Based on the One Component Linear Diffusion Model Implementation of Water Vapour Into Cellular Concrete Sample

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Abstract. This paper demonstrates the application of the inverse problem for calculating diffusion coefficient distribution into a porous cylindrical sample in a one-dimensional case. The work mainly aims to adapt a well-known diffusion equation with boundary conditions to obtain humidity profiles experimentally in porous samples. Empirical equations for diffusion coefficients according to humidity distribution are also reviewed. The main focus of this paper is concentrated on the proper interpretation of water vapour diffusion in coordinate and time dependencies. For this reason, the averaged quantities are introduced.

Keywords: porous media; inverse problem; water vapour diffusion; computation methods.

INTRODUCTION

Investigation of concrete ceramics is essential for understanding humidity migration into the porous media according to the classical behaviour of sorption isotherms or retention and drainage curves. It is well known [1] that the behaviour of the sorption curve according to experimental data [2] is reminded of the well-known Type IV sorption isotherms described by [4]. Also, work [1] demonstrated how the structural parameters of a porous body can be obtained according to drainage or retention curves. The primary purpose of this work refers to the calculation of diffusion properties of the water vapour component of the gas mixture in the porous sample of concrete-like composite ceramic under the condition that experimental data [2, 3] for distribution of water saturation corresponding to the pore saturation by liquid at isothermal condition is known from experimental or computer simulation data. This method, which refers to inverse mathematical problems, is first defined by the works [5, 6, 7] and classified as an ill-posed problem. Their solution does not satisfy the general requirements of existence, uniqueness and stability under small input data changes [8]. The inverse method has been used successfully to determine the thermal conductivity in heat conduction problems [9, 10]. Since the governing equations for heat conduction and moisture diffusion are the same, it is only natural to use the same procedure to investigate the diffusion coefficients in the cellular concrete ceramic's moisture resorption or desorption process. In all cases, the governing equations must be correctly formulated, and boundary and initial conditions must be used to fully describe the diffusion processes at the fixed external conditions into the environment.

Investigation object. Let's consider the porous cylindrical sample (Figure 1) of the height h, which is prepared on the base of cellular concrete. The sample was immersed in water until equilibrium hydration was reached under normal conditions.

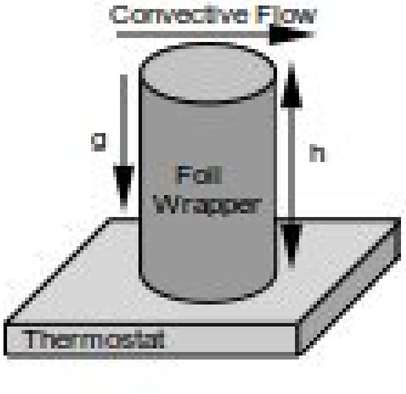

Figure 1 – Schematic representation of convective drying of the porous cylindrical sample

The lower plate surface of the cylindrical sample is tight and placed on the horizontal thermostat plate with a fixed temperature equal to the same value as the temperature of the ambient environment. The corner of the sample is wrapped in foil to prevent mass and heat transfer through the cylindrical surface. The upper surface is applied to the conditions of convective drying with a fixed value of the velocity of surface flows formed by hot air.

RESULTS AND DISCUSSION

Diffusion equation introduction

According to work [5, 6], the differential equation which describes the desorption or resorption phenomena into a porous sample of the water vapour component of the gas mixture in terms of a one-component linear diffusion problem at isothermal conditions may be represented in the form.

$$\frac{\partial C_v(z,t)}{\partial t} =$$
$$= \frac{\partial}{\partial z}\left(D(C_v;\phi,\tau)\frac{\partial C_v(z,t)}{\partial z}\right)(0 < z < h, t > 0), (1)$$

where $C_v(z,t)$ is the linear concentration of water vapour along $z$axis under (Figure 1) conditions of earth gravity, $D(C_v;\phi,\tau)$ is the varying in the coordinate z and time $t$diffusion coefficient of water vapour in the porous sample, ϕ and τ are the averaged porosity and touristy of the permeable body, h is the height of the porous sample.

Let the initial conditions be

$$C_v(z,t) = C_v^0\ (0\ "z"\ h, t = 0)$$

and boundary conditions look like

$$D(C_v;\phi,\tau)\frac{\partial C_v(z,t)}{\partial z} =$$
$$= \alpha[C_v^{env} - C_v(z,t)](z = h, t \geq 0),$$

where $\alpha$is the mass transfer coefficient, also named surface emission [7], C_v^0 and $C_v^{env}$are value of initial and external concentration of water vapor into ambient environment.

We assume that mass transfer under isothermal conditions may occur only in the radial direction perpendicularly to the sample's upper or lower horizontal surfaces (Figure 1).

We are considering the porous body as a component media consisting of the porous skeleton as a solid phase, non-adsorbed free water and a two-component gas mixture of water vapour and dry air into the porous space of the rigid skeleton. At this assumption, we can review [11, 12] the concentration of water vapour in porous media as a function of liquid pore saturation by relation

$$C_v = \phi(1 - \eta_W)\rho_v^G, \qquad (2)$$

where $\rho_v^G = p_v M_v / RT$ and $p_v = \varphi p_{vs}(T)$ are density and partial pressure of water vapour into the gas phase here $p_{vs}(T)$ is saturated water vapour pressure as a function only of thermodynamic temperature and $\varphi$is relative humidity of dry air in a porous sample.

We assume that the pore saturation by liquid $\eta_W = \eta_W(\varphi, T)$ is depends only on relative humidity and thermodynamic temperature. So, in general, we may represent the water vapour concentration in the form of a relation.

$$C_v = C_v(\eta_W) = C_v(\varphi, T). \qquad (3)$$

Below is the equal transformation of relation (2) according to assumed (3) assumption, which let's define

$$C_v = \phi[1-\eta_W(\varphi,T)]\frac{p_{vs}M_v(T)}{RT}\varphi. \qquad (4)$$

Also, it follows from Daltone's [12] law what $\rho_G = \rho_v^G + \rho_a^G$, here ρ_G is the gas phase density as a two-component non, non-interacted ideal mixture of water vapour and dry air. As was mentioned

$$\rho_G = \frac{1}{RT}[\varphi p_{vS}(T)M_v + \{P_G - \varphi p_{vS}(T)M_a\}], \qquad (5)$$

here M_v and M_a are the constant molar mass of water vapor and dry air in gas mixture.

It follows from above.

$$\rho_v = \varphi p_{vS}(T)M_v/RT \qquad (6)$$

and

$$\rho_a = (P_G - \varphi p_{vS}(T)M_a)/RT, \qquad (7)$$

here ρ_v and ρ_a are the partial densities of components of gas mixture.

Local averaging method

Accordingly to the method of local spatial averaging [13], let's define the total physical volume of averaging as

$$\Delta V_{SPL} = \Delta V_S + \Delta V_W + \Delta V_G, \qquad (8)$$

where ΔV_{SPL} is the elementary volume of averaging known as R.E.V (Representative Elementary Volume), ΔV_σ, here $\sigma = \{S, L, G\}$ is the index of solid (S) as a hard skeleton, liquid (L) as water and (G) as gas phases.

From relation (8), we can define local volumetric porosity as

$$\phi = 1 - \frac{\Delta V_S}{\Delta V_{SPL}} = \frac{\Delta V_W + \Delta V_G}{\Delta V_{SPL}}. \qquad (9)$$

Also, relative to (9), we can introduce the volume pores saturation by liquid and gas via relations.

$$\eta_W = \frac{\Delta V_W}{\Delta V_W + \Delta V_G} = \frac{\Delta V_W}{\phi \Delta V_{SPL}}$$

and $\eta_G = \frac{\Delta V_G}{\Delta V_W + \Delta V_G} = \frac{\Delta V_G}{\phi \Delta V_{SPL}}$ (10)

in such way that equality $\eta_W + \eta_G = 1$ is satisfied.

It is not hard to estimate that due to relation (9)-(10), we can represent the local quantity for the volumetric concentration of water in pores as:

$$\Delta C_W = \frac{\Delta m_W}{\Delta V_{SPL}} = \frac{\rho_W \Delta V_W}{\Delta V_{SPL}} = \phi \rho_W \eta_W, \qquad (11)$$

here ρ_W is constant density of water into the incompressible state. From the last relation, the local concentration of the gas phase takes a similar form.

$$\Delta C_G = \Delta C_v + \Delta C_a = \frac{\Delta m_G}{\Delta V_{SPL}} = \frac{\Delta m_v + \Delta m_a}{\Delta V_{SPL}} = \frac{\rho_G \Delta V_G}{\Delta V_{SPL}} = \phi \rho_G \eta_G.$$

Because $\rho_G = \rho_v^G + \rho_a^G$ and $\eta_W + \eta_G = 1$the equality (11) gives us the concentration of gas mixture component by the following relations

$$\Delta C_v = \frac{\Delta m_v}{\Delta V_{SPL}} = \frac{\rho_v \Delta V_G}{\Delta V_{SPL}} = \phi(1-\eta_W)\rho_v^G \qquad (12)$$

and

$$\Delta C_a = \frac{\Delta m_a}{\Delta V_{SPL}} = \frac{\rho_a \Delta V_G}{\Delta V_{SPL}} = \phi(1-\eta_W)\rho_a^G, \qquad (13)$$

where $\rho_v^G = p_v\, M_v/R\,T$ and $\rho_a^G = p_a\, M_a/R\,T$ is the partial density of water vapour and dry air in the gas mixture.

If isobaric conditions is satisfied, we can assume $\Delta V_v = \Delta V_a = \Delta V_G$, so the volume concentration of water vapour can introduced as

$$\Delta C_v = \phi(1-\eta_W)\rho_v^G$$
$$= \phi(1-\eta_W)\frac{p_{vS}(T)M_v}{RT}\varphi, \qquad (14)$$

here $p_v = \varphi p_{v_S}(T)$is a well-known relation, where $p_{v_S}(T)$ is the water vapour saturation pressure, and φ is the local quantity of relative humidity.

Comparing (12) with (3), we conclude that local value concentration has been defined previously properly or correctly. So, given the difference from equal equations (4, 13), we receive relations.

$$\frac{\partial C_\nu}{\partial z} = \phi \frac{p_{\nu s}(T) M_\nu}{RT}\left\{[1-\eta(\varphi)] - \varphi\frac{\partial \eta}{\partial \varphi}\right\}\frac{\partial \phi}{\partial z} - \phi[1-\eta(\varphi)]\frac{M_\nu}{RT}\left\{p_{\nu s}(T) - T\frac{\partial p_{\nu s}(T)}{\partial T}\right\}\frac{\varphi}{T}\frac{\partial T}{\partial z}, \quad (15)$$

here z is the coordinate into the above-mentioned differential form.

Negligible the last part differences in the equation above under isothermal condition we obtain

$$\frac{\partial C_\nu}{\partial X} = \phi\left\{[1-\eta(\varphi)] - \varphi\frac{\partial \eta}{\partial X}\right\}\frac{p_{\nu s}(T) M_\nu}{RT}\frac{\partial \phi}{\partial X}. \quad (16)$$

where the non-isothermal condition is considered, it is possible to represent equation (15) in the more general form

$$\frac{\partial C_\nu(z,t)}{\partial t} = D_\phi(\phi, T)\frac{\partial \phi(z,t)}{\partial z} + \frac{k_T(\phi,T)}{T}\frac{\partial T(z,t)}{\partial z}, \quad (14)$$

where

$$D_\nu(\phi, T) = \phi\frac{p_{\nu s}(T) M_\nu}{RT}\left\{[1-\eta(\varphi)] - \varphi\frac{\partial \eta(\varphi)}{\partial \varphi}\right\}$$

and

$$k_T(z,t) = \phi[1-\eta(\varphi)]\frac{M_\nu}{RT}\left\{p_{\nu s}(T) - T\frac{\partial p_{\nu s}(T)}{\partial T}\right\}\varphi$$

is the mentioned in (14) moisture diffusivity and thermo diffusion coefficient, respectively, in the case of the water vapour density slowly varying with temperature or, in other words, far from the temperature of phase transition.

General equations formulation

In general, under isothermal conditions, we may collect necessary relations [5, 6] for resolving a one-dimensional inverse problem in terms of water vapour concentration as a component of a gas mixture in such way:

I. Diffusion equation

$$\frac{\partial C_\nu(z,t)}{\partial t} = \frac{\partial}{\partial z}\left(D(C_\nu;\phi,\tau)\frac{\partial C_\nu(z,t)}{\partial z}\right)$$

$$(0 \leqslant z \leqslant h); \quad (15)$$

II. Boundary conditions

$$\frac{\partial C_\nu(z,t)}{\partial z} = 0 \; (z = 0, t \geqslant 0); \quad (16)$$

$$D(C_\nu;\phi,\tau)\frac{\partial C_\nu(z,t)}{\partial z} = \alpha\left(C_\nu^{eqv} - C_\nu\right). \; (z = h, t \geqslant 0$$

III. Initial conditions

$$C_\nu = C_\nu^0 \qquad (0 \leqslant z \leqslant h, t = 0), \quad (17)$$

May be considered as far as possible to possibilities: 1. $C_\nu^{eqv} > C_\nu$ is the desorption case; 2. $C_\nu^{eqv} < C_\nu$ is the sorption case, whereC_ν^{eqv} is the concentration of water vapour in the ambient environment, C_ν^0 is the corresponding to initial concentration at the zero time moment.

Empirical equations for diffusion coefficients

Let's focus on the known expressions in the literature [14, 15] for diffusion coefficients, which may be applied to the abovementioned relations (15). According to the ground of molecular-kinetic theory [14], the effective coefficient of molecular diffusion for water vapour or dry air in porous non-saturated media depends not only on the structural parameters of the material but also, according to [15] equation on temperature and dynamical viscosity components of the gas mixture. The works [16,17] review a half empirical relation for such diffusion coefficient in a two-component mixture's standard temperature and total pressure interval. It can also be applied to describing the drying process under convective conditions.

For illustration of transport properties of water vapour or dry air in the porous sample, the classical Burger [19] diffusion coefficient is used by the following expressions

$$D_P = \frac{\theta(z,t)_\alpha}{k - \theta(z,t)_\alpha(k-1)} D_\alpha^\beta, \quad (18)$$

where D_P is diffusion coefficient of α-component into the porous skeleton and D_α^β is mutual diffusion coefficient for α-component of the mixture ($\alpha = \nu$ is water vapour) into a β-component of the mix ($\beta = a$ is dry air) accordingly,θ_α is the volume fraction of diffusion components, and k is the constant structure parameter, so the diffusion coefficient looks like

$$D(z,t) = \frac{1}{\tau} D_P = \frac{1}{\tau} f_s D_v^a, \tag{19}$$

where

$$f_s = \langle\varphi\rangle(1-\eta_L)/[\kappa - \langle\varphi\rangle(1-\eta_L)(1-\kappa)]$$

is a correction to diffusion joined with wetting of pores, D_v^a is the diffusion coefficient of water vapour in dry air, τ is the tortuosity factor and $\kappa$is an unknown parameter which characterizes the properties of the porous material.

According to the [20] model, it is possible also define the effective diffusion coefficient D_P for α-component in the pore of investigated material as

$$D_P = \frac{\theta_\alpha^{10/3}}{\langle\varphi\rangle^2} D_\alpha^\beta, \tag{20}$$

here D_α^β is the coefficient of mutual diffusion for α-component (water vapour) into β-component (dry air) and θ_α is the volume fraction of α-component for diffusion, from it is follows

$$D_P = \langle\varphi\rangle^{4/3}(1-\eta_L)^{10/3} D_v^a, \tag{21}$$

here D_v^a is the mutual diffusion coefficient of water vapor into the dry air.

Relative velocity of gas mixture component u_v^x and u_a^x according to the definition of molecular Fick's [18] diffusion flow, changing during porous material wetting is also essential. So, for components of a gas mixture on the cross surface of porous material by meaning [20] (20) diffusion coefficient, it is possible to select the effective constituent of diffusion D_S^v and D_S^a for water vapour (v) and dry air (a) components accordingly. In such case

$$D(z,t) = \frac{1}{\tau} D_P \equiv \bar{D_v} \equiv \bar{D_a}, \tag{22}$$

$$\bar{D_v} = \frac{\langle\varphi\rangle}{\tau} D_P^v, \quad \bar{D_a} = \frac{\langle\varphi\rangle(1-\eta_L)}{\tau} D_P^a, \tag{23}$$

where $\frac{1-\eta_L \square^{10/3} D_v^a}{D_P^v = \langle\varphi\rangle^{1/3}}$ and $\frac{1-\eta_L \square^{7/3} D_v^a}{D_P^a = \langle\varphi\rangle^{1/3}}$

is constituted of diffusion coefficient by water vapour (v) and dry air (a) into the dewy porous material.

The empirical approaches corresponding to mathematical relations (19) and (23) unfortunately can not describe the entire distribution of diffusivity in the coordinate z and time t in the case of when the dynamic changes of humidity $\varphi = \varphi(z,t)$, temperature $T = T(z,t)$ or pressure $P_G = P_G(z,t)$ Profile in porous media is known from experimental data or obtained from numerical simulations. So, resolving the inverse problem to get the diffusion coefficient distribution in the porous sample is one of the main essential methods to determine the diffusivity properties of the investigated porous material. We will consider the necessary steps to mathematically resolve the inverse diffusion problem in the following sections of this paper.

Numerical approaches for finite difference method

The main idea introduced by the works [5-7] in the inverse method is searching for diffusion coefficients in equations (15-17). It consists of the numerical resolution of the differential equation (15) using the finite difference method.

For this purpose, let half specimen heath of h to be discretized with mesh with Δzin the space and Δt in the time direction with grid points for coordinate $\Delta z_j = j\Delta z$(where $j = 0,1,\ldots,n$) and time $t_i = i * \Delta t$(where $i = 0,1,2,\ldots$). The procedures described below will assume that $C_v(z,t)$are known at grid points $\{z_j, t_i\}$.

According to the finite difference method, the numerical solution of the diffusion equation (15) in the matrix form looks like

$$\hat{A} d = b, \tag{24}$$

where $\hat{A}$ is the three-diagonal square matrix

$$\hat{A} = \begin{bmatrix} a_{0,0} & a_{0,1} & . & . & . & . & . \\ a_{1,0} & a_{1,1} & a_{2,1} & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ . & . & . & . & a_{n-1,n-2} & a_{n-1,n-1} & a_{n-1,n} \\ . & . & . & . & . & a_{n,n-1} & a_{n,n} \end{bmatrix} \tag{25}$$

also $d = \begin{bmatrix} d_0 \\ \cdot \\ \cdot \\ \cdot \\ d_n \end{bmatrix}$ and $b = \begin{bmatrix} b_0 \\ \cdot \\ \cdot \\ \cdot \\ b_0 \end{bmatrix}$

are the vectors of unknown diffusion coefficient values and time derivatives from water vapour concentrations.

a. At the upper surface greed point with $z = z_0$ and $t = \bar{t}$we have

$$a_{0,0} = \left[\begin{array}{c} 2C_v(z_{0,}\bar{t}) - \\ 3C_v(z_{1,}\bar{t}) + C_v(z_{2,}\bar{t}) \end{array}\right] / \Delta z^2,$$

$$a_{0,1} = \left[-C_v(z_{0,}\bar{t}) + C_v(z_{1,}\bar{t})\right] / \Delta z^2, \qquad (26)$$

$$b_0 = \left[\begin{array}{c} C_v(z_{0,}\bar{t} + \Delta t) - \\ C_v(z_{0,}\bar{t} - \Delta t) \end{array}\right] / 2\,\Delta t;$$

b. At the internal grid point with

$z = z_j (0 < j < n)$ and $t = \bar{t}$we have

$$a_{j,j-1} = \left[C_v(z_{j-1}, \bar{t}) - C_v(z_{j+1}, \bar{t})\right] / \Delta z^2,$$

$$a_{j,j} = 4\left[\begin{array}{c} C_v(z_{j+1}, \bar{t}) - \\ 2C_v(z_j, \bar{t}) + C_v(z_{j-1}, \bar{t}) \end{array}\right] / \Delta z^2, \qquad (27)$$

$$a_{j,j+1} = \left[\begin{array}{c} C_v(z_{j+1}, \bar{t}) - \\ C_v(z_{j-1}, \bar{t}) \end{array}\right] / \Delta z^2,$$

$$b_j = 2\left[\begin{array}{c} C_v(z_j, \bar{t} + \Delta t) - \\ C_v(z_j, \bar{t} - \Delta t) \end{array}\right] / \Delta t;$$

c. At the lower grid point with $z = z_n$ and $t = \bar{t}$we have

$$a_{j,j} = 2\left[\begin{array}{c} C_v(z_{n-1}, \bar{t}) - \\ C_v(z_n, \bar{t}) \end{array}\right] / \Delta z^2, \qquad (28)$$

$$b_n = \left[\begin{array}{c} C_v(z_n, \bar{t} + \Delta t) - \\ C_v(z_n, \bar{t} - \Delta t) \end{array}\right] / 2\,\Delta t.$$

As was mentioned in works [6, 7], the small changes in vector b may result in significant changes in the numerical solutions by finite-difference equations (25-27) depending on the degree of the ill-conditioning property of the three-diagonal matrix (24). Therefore, accurate data generation can not be overemphasized when applying the inverse technique.

The input data for the computation of the inverse diffusion problem

The works [3] obtained the primary experimental data for the classical building material, cellular concrete ceramic. The experimental or numerical results have been determined in the porous cylindrical (Figure1) sample of height $h = 0.01[m]$ with averaged porosity $\phi = 0.70$ and tortuosity factor $\tau = 4$ under averaged (Figure 2, right image) constant temperature $T = 301.5(K)$. The external environment outside the sample was supported by continuous room temperature $T_{amb} = 320.15[K]$ and normal ambient $P_G = 101325[Pa]$ atmospheric pressure. For numerical simulation in the work [3] on the upper surface, it was suggested to put the constant mass $\alpha = 0.015[m/c]$ and heat ($\beta = 15[W/(m^2K)]$) transfer coefficients by the mentioned numbers under ideal ($\varphi = 0 | z \to \infty$) drying conditions.

Let's review (Figures 2 and 3) the computer simulation results of heat and mass transfer due to work [3] under convective drying conditions of the horizontal cylindrical porous sample prepared on the base of cellular concrete ceramic.

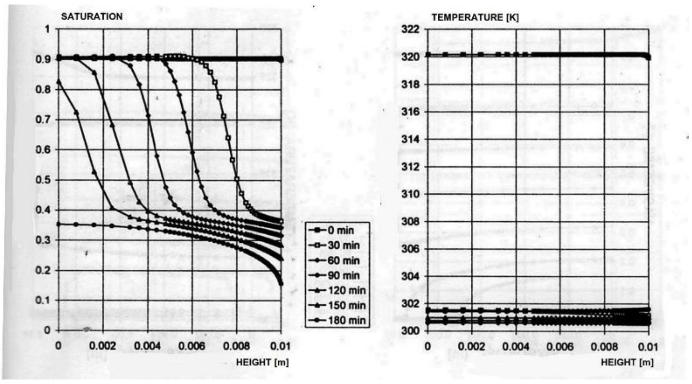

Figure 2 – Depiction of computer simulation results for cellular concrete, ceramic cylindrical sample in terms of pore saturation by liquid (left image) and temperature (right image) as a function of sample height

As depicted (Figure 2, left image), the classic example of pore saturation by a liquid relative to the sample height was received, not critical change temperature (Figure 2, right image) profile under drying conditions. The gas pressure profile was also reproduced during computer simulation [3] (Figure 3).

It follows from such results of computer simulation of the drying process that the thermodynamic state of the gas mixture can be reviewed under near isothermal and isobaric conditions, so dependencies.

$T = T(z, t)$ and $P_G = P_G(z, t)$, in general, can be neglected.

Of course, work [3] has resolved a more general problem [11, 12] when the diffusion equation describes moisture and temperature transport. The limitation of using such equations [12], which are similar from a mathematical point of view, is the correct definition of heat sources and evaporation rate.

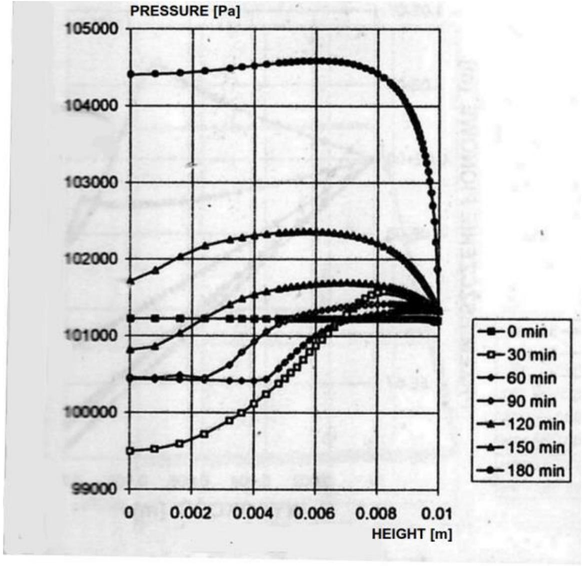

Figure 3 – Depiction of computer simulation results for cellular concrete and ceramic cylindrical samples regarding gas pressure as a function of sample height

Because it is outside of this paper, we may assume that the same dependence of pressure for gas mixture exists due to the evaporation of water into the pores of the sample. Still, the changes in pressure, as shown in Figure 3, are not essential for the mentioned porous material under convective drying conditions. The thermal effects due to evaporation, which are reviewed in work [3] not only as a source of heat but also as by hydration or dehydration enthalpy change is also neglected in this paper according to an assumption that main transport (Figure 2) on the body surface is moisture diffusion.

The main distribution (Figure 2, left image) obtained during the described work [3] computer simulation can be transmitted to the form of relation (Figure 4, it is the second curve from the left side of the selected material) between pore saturation by liquid η_L and effective radius $\bar{r}$ of pores ($\eta_L = \eta_L(\bar{r})$ as depicted below.

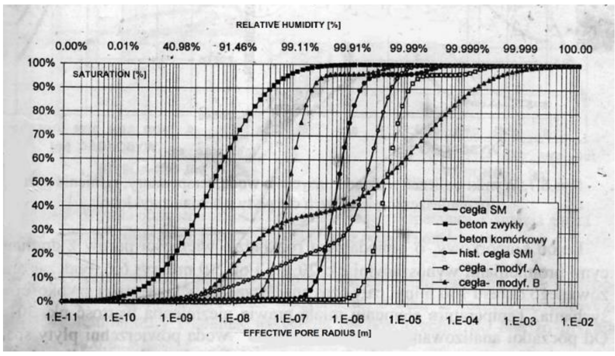

Figure 4 – Depiction of computer simulation results for cellular concrete, ceramic cylindrical sample in terms of gas pressure as a function of sample height

here $\bar{r} = 1/R_1 + 1/R_2$ is defined by radii $R_1$and $R_2$to the averaged meniscus between the water and gas phase in radial and tangential directions [4] correspondingly) from which we can obtain by [4] relation $\phi = exp[-(M_v \rho_L RT)/(2\,\sigma/r)]$ more general dependence $\eta_L = \eta_L(\phi)$ as it's depicted below.

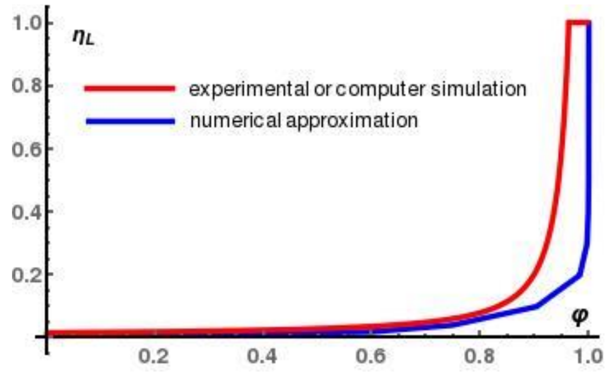

Figure 5 – The central dependence of pore liquid saturation by water from the relative humidity of dry air and air-gas mixture

Using the first good approximation by the relation

$$a_0(1-x) + b_0/(1-x) + c_0/(1-x)^2 + d_0/(1-x)^4 \qquad (29)$$

where $a_0 = -0.015$, $a_0 = 0.015$, $b_0 = 0.000001$and $d_0 = 0.0000001$ is the constant numerical parameter we can reproduce (Figure 2, left image) corresponding to the coordinate (Figures 6 and 7) relation for the distribution of pore saturation by liquid.

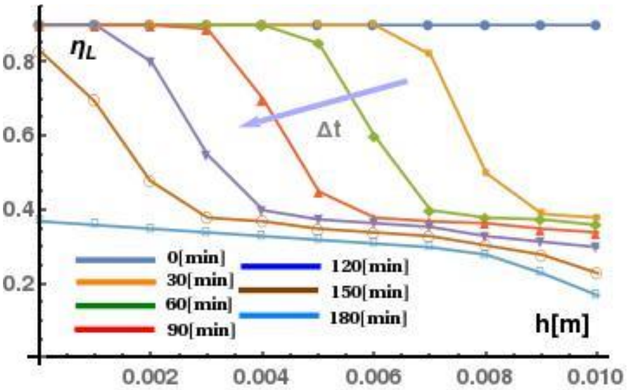

Figure 6 – Dependence of pore liquid saturation by water from a height of porous sample

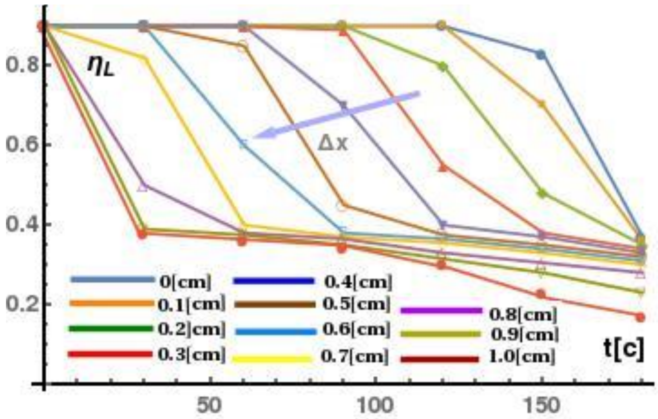

Figure 7 – Dependence of pore liquid saturation by water from time of drying at various horizontal surfaces of the porous sample according to coordinate greed points

It is important to remark that the initial value of pore saturation by liquid is not essential for the numerical solution of inverse problems. So, the same mistake in the approximation relation (29) is possible (Figure 1) within reason.

From obtained via experimental or numerical data [3] approximation (29), it is easy to estimate averaged over time and coordinate graphs according to the procedure of discretization in the time $\Delta t = 30(\text{min})$ and space $\Delta z = 0.01(\text{m})$ intervals.

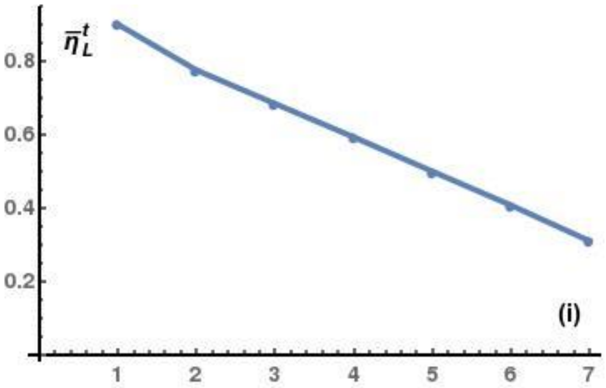

Figure 8 – Dependence of averaged by time pore saturation by liquid on the time-space greed

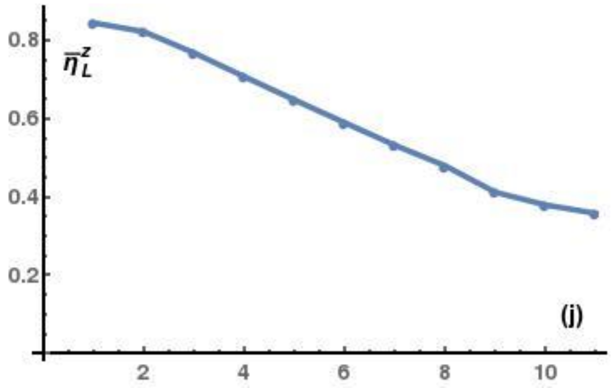

Figure 9 – Dependence of averaged by coordinate pore saturation by liquid on the coordinate space coor greed

Numerical analysis of experimental data

From the experimental or numerical simulation data [3] (Figure 3), we also can obtain what, averaged by the height of the sample, the total pressure of the gas mixture (Figure 10) really can not change significantly.

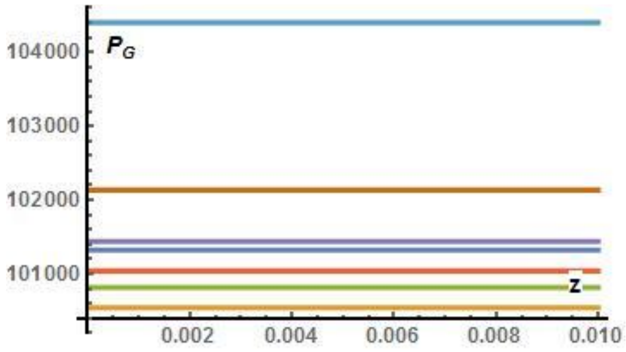

Figure 10 – Changes averaged by the height of sample total pressure during the drying process

So, under usage, the average value of total pressure $P_G = 101672[kPa]$ we have, according to (12)-(13), the following graphical dependencies (Figures 11 and 12) for the concentration of water vapour and dry air in the porous sample, which follows from the essential known dependence (Figure 5) of pore saturation by liquid from relative humidity.

As depicted in Figures 11 and 12 below, there is a natural behaviour of dependencies according to which the concentrations of water vapour increase and dry air decreases with a magnification of relative humidity. Let's denote that in the vicinity close to the saturation value of relative humidity, the concentration of water vapour is decreasing strongly, which may be due to processes of condensation of water vapour.

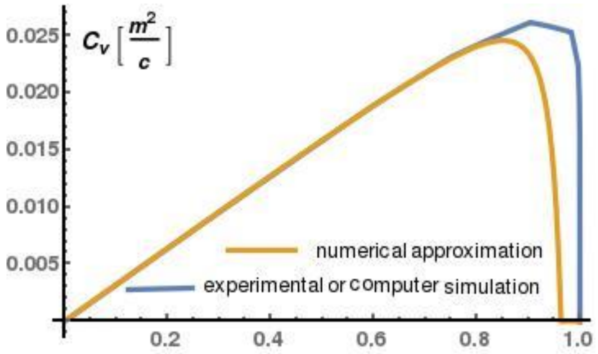

Figure 11 – Concentration of water vapour as a function of relative humidity

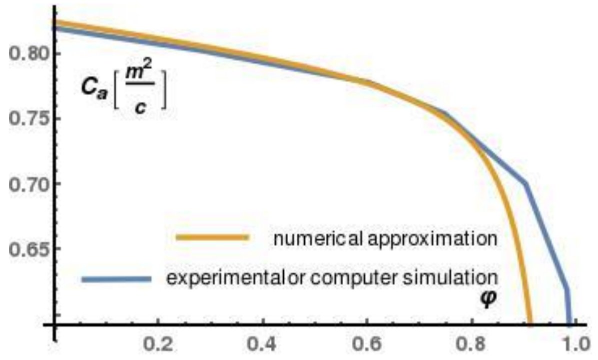

Figure 12 – Concentration of dry air as a function of relative humidity

Based on the general dependence (Figure 5) with the usage of experimental data and approximation by relation (29), we can illustrate the theoretical approaches for diffusion coefficients into the [19] ((18)-(19)) or [20] ((21)–(22)) representation in the denotation of water vapour and dry air (23) respectively. The results can be obtained through simple calculations, as depicted in Figures 13 and 14.

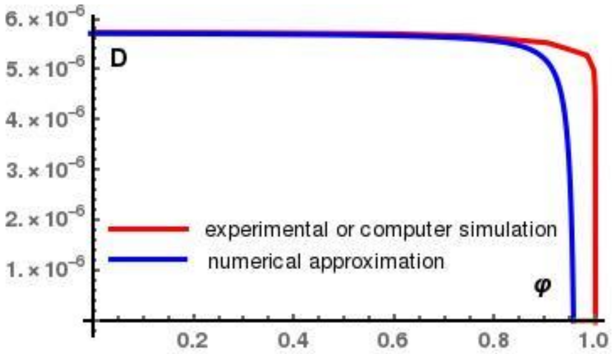

Figure 13 – Theoretical approach for [19] diffusion coefficient at $\kappa = 0.28$ delivered by experimental date and numerical approximation.

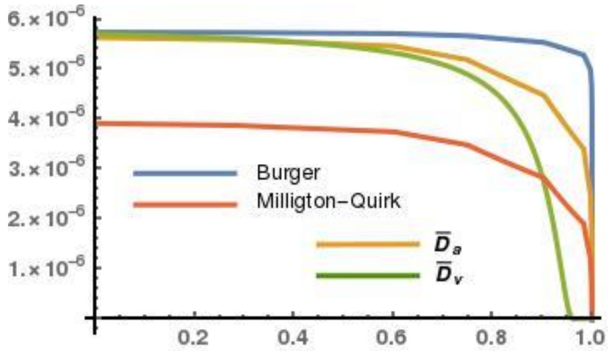

Figure 14 – Theoretical approach for [20] diffusion coefficient by effective constituents of dry air ($\alpha = a$) and water vapour ($\alpha = v$) for gas mixture components

To compare different theoretical diffusion approaches, we collect the phenomenological graphical relations based on the [19, 20] diffusion models in one graph (Figure 15), as shown below.

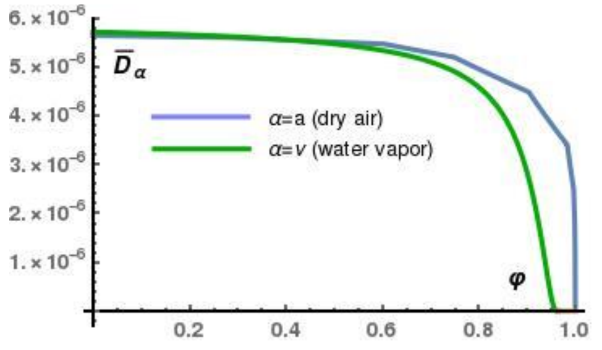

Figure 15 – Comparison between different theoretical phenomenological models for a description of the diffusion coefficient into porous media

Let's stop on the central relations for averaged over the time (Figure 16) and space (Figure 17) diffusion coefficient defined by [19], which, due to the graphical representation of average over time (Figure 8) and coordinate (Figure 9) pore saturation by liquid looking as

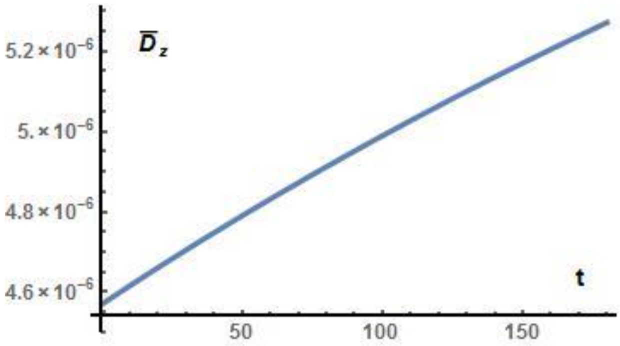

Figure 16 – Averaged over time, the theoretical diffusion coefficient as a function of time

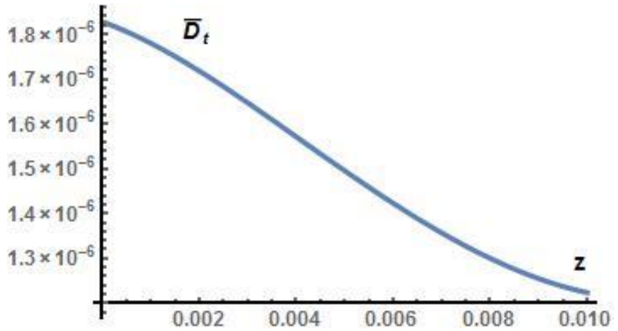

Figure 17 – Averaged over coordinate the theoretical diffusion coefficient as a function of coordinate.

The picture below does not claim to be complete because an empirical relation was used for the diffusion coefficient (19), which does not point to the natural process of humidity migration into porous samples. It was obtained from experimental or numerically simulated data [3], in which the assumption of isothermal conditions generally have a form depicted in Figures 6 and 7 for coordinate and time distributions, respectively. This relation can not reflect the distribution of the absolute diffusivity value in a porous body because it was aligned to known empirical models for diffusion coefficients, as shown in Figure 15 in the previous graphs.

At the end of this section, let's demonstrate (Figure 18) the average over-height of the sample change of relative humidity from drying.

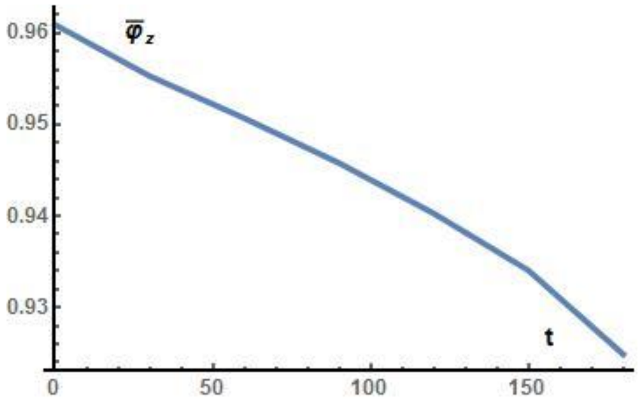

Figure 18 – Change of averaged over the height of sample humidity in tine

As a result of extrapolation of essential relation $\eta_L = \eta_L(\bar{r})$[3] (Figure 2, left image) for relative changes of pore saturation by liquid from averaged liquid meniscus radios.

Numerical solution of inverse diffusion problem

Just now is the time to understand the scientific material demonstrated above to outline the main results of this paper. For this purpose, we demonstrate a numerical solution of matrix (24) using the numerical data described below in the following graphical relation.

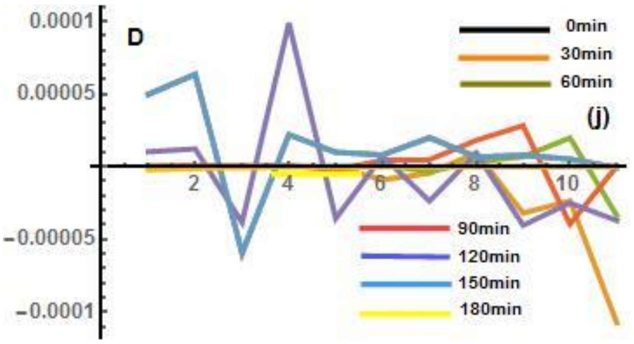

Figure 19 – Solution of the inverse problem for diffusion coefficient as a function of height of sample into the coordinate greed point at different points of time

From the first point of view, it is something incomprehensible. A question immediately arises: perhaps something is wrong with the selection of the coordinate axis? However, look at the graphs (Figures 20 and 21) below in a different view according to the abscissa.

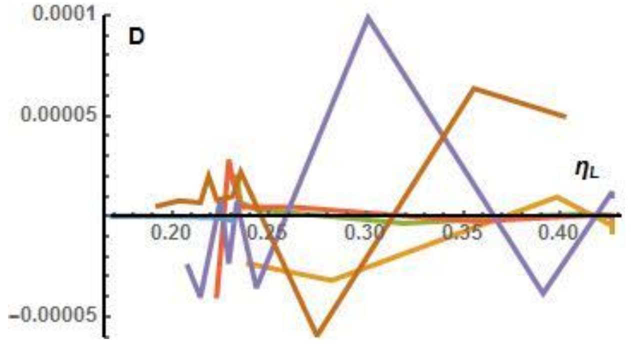

Figure 20 – Solution of the inverse problem for diffusion coefficient as a function of pore saturation by liquid of sample at different points of time

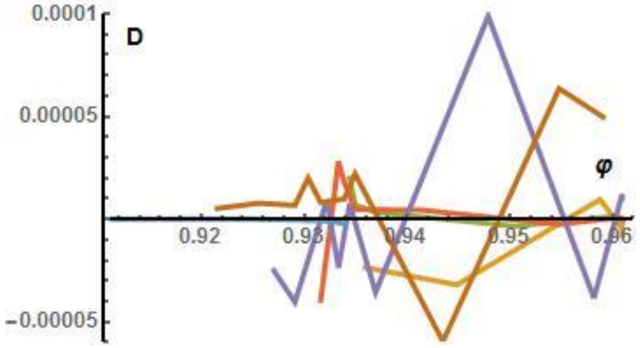

Figure 21 – Solution of the inverse problem for diffusion coefficient as a function of relative humidity of the sample at different points in time

It follows from the above groups (Figures 19, 20, 21) graphical dependencies that local averaged [13] mesoscopic properties of porous media are unsuitable for describing the diffusion properties of a porous sample in macroscopic (15-17) diffusion equations.

To adequately describe macroscopic diffusivity properties of porous media, it must average over time or coordinate the shoved below dependencies. Based on known graphs (Figures 19, 20, 21), we receive the complete solution of the inverse diffusion model in the form.

The inverse problem (Figures 22 and 23) for searching for diffusion coefficient in a humidified porous sample can be considered fully resolved.

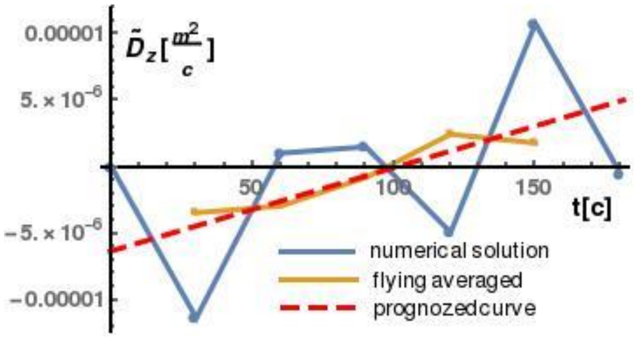

Figure 22 – Averaged over the sample diffusion coefficient height as a time function

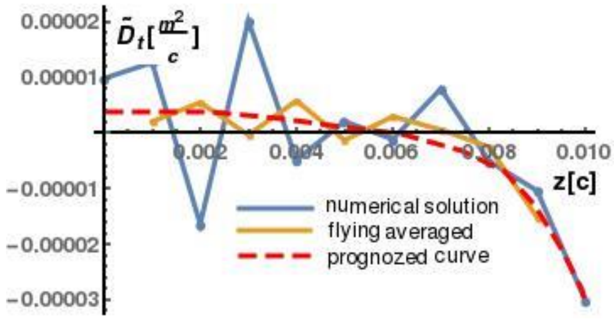

Figure 23 – Averaged over time of drying diffusion coefficient as a function of the height of the sample

CONCLUSIONS

The main conclusion in this paper can be received with an understanding of the proposed logical chain. First, we must know or obtain in another version the uniqueness of Lets emphasize that this is not unique and is also an essential macroscopic characteristic of a porous body. Second, one-dimensional equations due to the local averaging method can only be considered in terms of relative humidity distribution in porous bodies. The input data in resolving inverse diffusion problems (25) can be obtained by concentration profiles (12)-(13), as it is shown in Figures 11 and 12, respectively. Third, the obtained by of the ill-conditioning property of the three-diagonal matrix (25) distribution of the diffusion coefficients through time and coordinate can not sense into the macroscopic scale, so only averaged quantities of diffusion coefficients can be applied to macroscopic (15-17) diffusion equations. There is also an exciting effect in the limitation of diffusion coefficient values (Figures 20 and 21) near small values of liquid saturation, which corresponds to the existence of the lover limit of humidity into pores due to the starting of the adsorption process or existing residual saturation [1] in the form of adsorbed water. The change of sign is not entirely justified in the averaged quantities of diffusion coefficients but may correspond to the opposite action of suction and gravity effects. With limited access to complete experimental data, the averaged results (Figures 22 and 23) are not as plain as you would like. However, this work solves the general problem of equalizing a porous body's corresponding input physical characteristics in the diffusion equations in the first approximation.

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