

# Modeling and Investigation of the Effect of Diffusion and Mass Transfer in Capillary-Porous Bodies

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**Abstract** –A complex of issues related to the occurrence of physical processes during the formation of the necessary technological parameters, in particular, the effect of anomalous diffusion, is considered. On the example of energy systems for ensuring the microclimate of buildings with windows of increased tightness, the influence of diffusion is investigated and the results of modeling and research of heat and air exchange modes in a building with windows of increased tightness, obtained using the original mathematical apparatus and software, are presented. It is shown that the real savings in thermal energy, provided by the introduction of windows with increased tightness, is reduced due to latent heat losses associated with an increase in the ventilation load to ensure a comfortable microclimate. The conditions and ways of the most complete realization of technical and economic advantages from the use of windows of increased tightness are proposed.

**Keywords** – modeling, automation, energy system, heat and mass transfer, efficiency

## I. INTRODUCTION

Considerable attention of researchers and developers has been attracted to the issues of modeling and studying the effect of diffusion and mass transfer in capillary-porous bodies for energy saving and energy efficiency in energy systems, in particular, microclimate problems can be singled out. Research centers in Germany, Norway, USA,

Australia, France and Russia are engaged in developments in this area. At the same time, automated control of systems, taking into account the above physical processes, makes an additional contribution to energy efficiency.

The article considers the heat consumption management system of a public building with various rooms with different technological, which, in addition to providing real cost savings on microclimate provision, makes it possible to identify and investigate the patterns of functioning of energy-efficient buildings and analyze the effectiveness of individual energy-saving measures. As such an event, the building is considered to be equipped with windows of increased tightness. The preliminary results of this analysis have already shown that due to changes in the mass transfer flows in the indoor-outdoor air system, the existing microclimate systems are often not ready to bear the increased ventilation load due to window sealing. The results of direct measurement of regulated microclimate indicators in the premises of the building, equipped with windows of increased tightness, revealed peak excesses of the permissible carbon dioxide content and the level of comfortable temperature, a decrease below the permissible level of indoor air mobility. The consequence of this (in addition to the discomfort of people) is the growth of latent heat losses, and the benefits from the use of windows with increased tightness, as well as from the previously introduced automated heat consumption control system, are not fully realized.

To study the conditions and ways to improve the efficiency of energy systems for providing the microclimate of buildings with windows of increased tightness, a special study was undertaken, the results of which are devoted to the material of this article.

## II. PROPOSED ALGORITHM

### A. Problems of mass transfer in buildings –

To simulate the heat transfer of a building, we used the previously developed mathematical apparatus and the software product that implements it, taking into account the effect of high-tightness windows on the heat balance. The heat balance of an individual room or building as a whole consists of the following components:

$$Q_1 + Q_2 + Q_3 + Q_4 = Q_5 + Q_6 + Q_7, (1)$$

where  $Q_1$  is the heat output of the heating system, W;  $Q_2$  - total thermal power of lighting fixtures, W;  $Q_3$  – heat input from people, W;  $Q_4$  – heat input due to insolation, W;  $Q_5$  - heat losses due to heat transfer through the building envelope, W;  $Q_6$  – heat losses associated with outdoor air infiltration, W;  $Q_7$ ;- heat losses associated with the ventilation of the room, W

Monitoring of the thermal state of the building, performed during the heating period (before equipping windows with increased tightness), showed that up to 60% of losses occur in  $Q_5$  and at least 40% occur in  $Q_6$  and  $Q_7$ . The introduction of windows with increased tightness affects the  $Q_6$  component of the heat balance, reducing it to almost zero, and indirectly affects the  $Q_1$ ,  $Q_4$  and  $Q_7$  components. It is precisely because of the indirect influence that the real savings in thermal energy, provided by the introduction of windows with increased tightness, turn out to be significantly less than expected.

Let us consider the features of this influence in more detail. If  $Q_1$  is not adapted to the change in  $Q_6$ , this will lead to an increase in temperature. So, after equipping the main educational building with windows of increased tightness, the temperature in the rooms exceeded the comfortable level by an average of 5–6 °C [2]. The consequence is an increase in latent heat losses due to ventilation of the premises, which negates the positive effect of reducing  $Q_6$ . Therefore, it is obvious that it is possible to realize the benefits of using windows with increased tightness only if  $Q_1$  is correspondingly reduced. One of the options is the introduction of automated systems for managing the heat consumption of buildings based on its regulation by time of day, facades and floors of the building

The indirect influence of these windows on the  $Q_7$  balance (1) is an increase in the load on ventilation at zero infiltration of the outside air. The additional load on ventilation is determined by the permissible concentrations of harmful substances. In most premises of public and residential buildings, air exchange is provided by a general exchange natural ventilation system, which functions due to the inflow of outside air through leaks in window structures and its removal through exhaust ducts. For such premises, the energy system of the microclimate must ensure the removal of excess heat, moisture and carbon dioxide  $CO_2$ . So, with regard to  $CO_2$ , the additional flow rate of air removed from the room can be calculated by the formula:

$$\Delta G_v = \frac{G_{CO_2}}{n_2 - n_1} - G_{v,0} \quad (2)$$

where  $G_{CO_2}$  – is the volumetric flow rate of carbon dioxide released in the room,  $cm^3/h$ ;  $n_1$  and  $n_2$  – allowable concentrations of carbon dioxide in the outdoor air and in the indoor air,  $cm^3/m^3$ ;  $G_{y,0}$  – volumetric performance of the existing ventilation system in the room,  $m^3/h$ .

The balance of excess heat, moisture and carbon dioxide in the room is described by the following equations:

$$Q_{II} + \sum_{i=1}^n G_{II_i} \cdot I_{II_i} - \sum_{j=1}^m G_{y_j} \cdot I_{y_j} = 0 \quad (3)$$

$$M_{ea} + \sum_{i=1}^n G_{II_i} \cdot d_{II_i} \cdot 10^{-3} - \sum_{j=1}^m G_{y_j} \cdot d_{y_j} \cdot 10^{-3} = 0 \quad (4)$$

$$M_{CO_2} + \sum_{i=1}^n G_{II_i} \cdot \frac{c_{II_i}}{\rho_{II_i}} - \sum_{j=1}^m G_{y_j} \cdot \frac{c_{y_j}}{\rho_{y_j}} = 0 \quad (5)$$

where  $Q_{II}$  – is the excess heat released in the room, J/h;  $G_{II_i}$ ,  $G_{y_j}$  – respectively, the consumption of supply and exhaust ventilation systems in the room, kg/h;  $I_{II_i}$ ,  $I_{y_j}$  – respectively, the enthalpy of supply and exhaust air;  $M_{ea}$  – moisture released in the room, kg/h, кг/ч;  $d_{II_i}$ ,  $d_{y_j}$  – respectively, the degree of dryness of the supply and exhaust air, g/kg;  $M_{CO_2}$  – carbon dioxide released into the room, l/h;  $c_{II_i}$ ,  $\rho_{II_i}$ ,  $c_{y_j}$ ,  $\rho_{y_j}$  – are the concentration and density of the supply and exhaust air, respectively.

By solving equations (3)-(5) we obtain the amount of air required to dissipate excess harmful substances:

$$\Delta G_{II} = \frac{Q_{II}}{I_{y_j} - I_{II_i}} \quad (6)$$

$$\Delta G_{ea} = \frac{M_{ea}}{(d_{y_j} - d_{II_i}) \cdot 10^{-3}}, \quad (7)$$

$$\Delta G_{CO_2} = \frac{M_{CO_2}}{(n_2 - n_1) \cdot 10^{-3}} \quad (8)$$

Since there is no infiltration of outside air. The consequence of this is the impossibility of the entry of oxygen  $O_2$  into the room and the dispersion of carbon dioxide  $CO_2$ . The way out of this situation is to create conditions for diffusion transfer through the external enclosing structures, which are capillary-porous bodies and through a special valve in the external enclosing structures, created to increase the diffusion process.

#### B. Diffusion in capillary-porous bodies –

The classical description of diffusion processes is based on Fick's laws. A consequence of the second law is the classical differential diffusion equation:

$$J = -DS (\partial C / \partial x) \quad (9)$$

where S is the surface area of the area through which diffusion occurs.

In recent years, there has been an increased interest in the study of diffusion processes that do not obey Fick's laws and are not described by a classical equation. Transport phenomena that do not fit into classical concepts are observed, for example, in turbulent flows, in amorphous semiconductors, high-energy plasmas, and porous media. These phenomena are called anomalous diffusion.

An analysis of diffusion in a complex medium shows that the usual diffusion equation based on Fick's law cannot model the anomalous nature of diffusion mass transfer observed in field and laboratory experiments. New mathematical models of diffusion transfer, different from Fick's law, have been proposed and confirmed in the literature.

Anomalous diffusion generalizes normal diffusion in the case of considering processes in inhomogeneous and turbulent media. Anomalous diffusion processes are characterized by a power-law dependence of the diffusion packet width on time:

$$\Delta x \propto D_a t^y \quad (10)$$

Depending on the value of the exponent  $\gamma$ , different modes of diffusion are distinguished: in the case when  $\gamma > 1/2$ , we are dealing with superdiffusion, and with  $\gamma < 1/2$ , with subdiffusion. If  $\gamma = 1/2$  is normal diffusion.

The anomalous diffusion model is based on the continuous-time random walk model (CTRW). This model describes the wandering of a particle using a hop-trap mechanism. Particle walk is a sequence of instantaneous random jumps of value  $R_i$ ,  $i=1,2,3,\dots$  and rest states with random rest times  $T_i$ ,  $i=1,2,3,\dots$ . Jump values  $R_i$  are independent random variables and have distribution  $p(x)$ . The rest times  $T_i$  are also independent random variables both among themselves and on the sequence  $R_i$  and are distributed with a density  $q(t)$

### III. EXPERIMENT AND RESULT

Due to the lack of infiltration in indoor air, harmful substances accumulate. On fig. 1 presents some results of experimental changes in the concentration of carbon dioxide in the air in one (representative) auditorium of a building with windows of increased tightness.

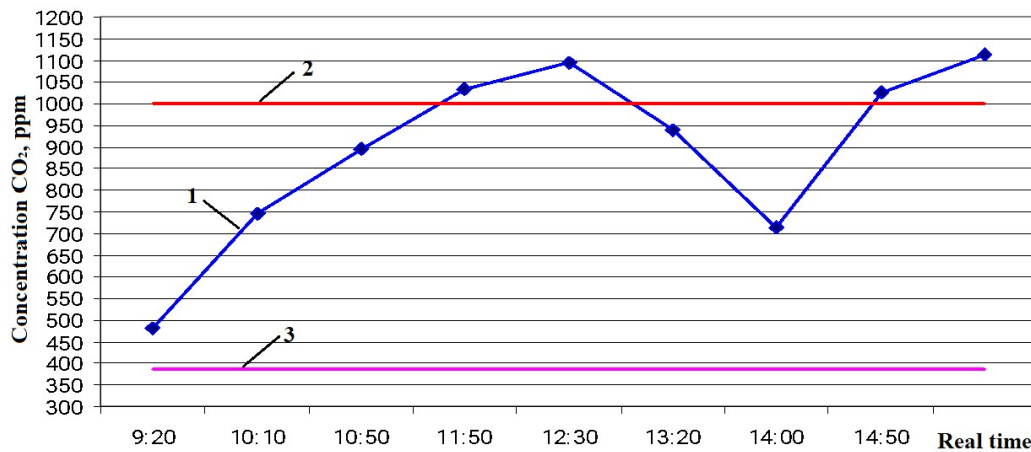


Figure 1. Changes in the concentration of carbon dioxide in an auditorium with windows of increased tightness: 1 - experiment; 2, 3 – the concentration of carbon dioxide, respectively, the maximum permissible and in fresh air ( $n_1 = 1000 \text{ cm}^3/\text{m}^3$ ,  $n_2 = 380 \text{ cm}^3/\text{m}^3$ )

To stabilize the microclimate parameters, it is necessary to determine the optimal diffusion parameters. The model of continuous random walk in time underlies the model of anomalous diffusion. The random walk of a particle is a sequence of instantaneous random jumps in the magnitude of the rest state with random rest times, which successively replace each other.

The continuous-time random walk model, which underlies the anomalous diffusion model, is described by the integral transport equation.

Equation (10) describes one-dimensional walks of a particle in the process of random walks with continuous time

$$\rho(x, t) = \frac{1}{v_0} \int_0^{v_0 t} P(\xi)(w_1 s(x - \xi, t - \xi / v_0) + (w_2 s(x + \xi, t - \xi / v_0))) d\xi + \int_0^{v_0 t} p(\xi)(w_1 \rho(x - \xi, t - \xi / v_0) + (w_2 \rho(x + \xi, t - \xi / v_0))) d\xi \tag{11}$$

The solution of equation (11) is found by the standard Fourier–Laplace transform method:

$$\hat{\rho}(k, \lambda) = \frac{1}{v_0} s_2(k, \lambda)(w_1 \hat{P}(\lambda/v_0 - ik) + w_2 \hat{P}(\lambda/v_0 + ik)) + \hat{\rho}(k, \lambda)(w_1 \hat{p}(\lambda/v_0 - ik) + w_2 \hat{p}(\lambda/v_0 + ik)) \tag{11}$$

here  $q(\lambda)$  is the Laplace transform of the density  $q(t)$ ,  $p(k)$  is the Fourier transform of the density  $p(\xi)$ ,  $s_1(k, \lambda)$  is the Fourier-Laplace transform of the original function  $s_1(x, t)$ .

A graphical solution using some methods of stochastic solution of the anomalous diffusion equation with a fractional derivative both in time and coordinate is shown in Fig. 2.

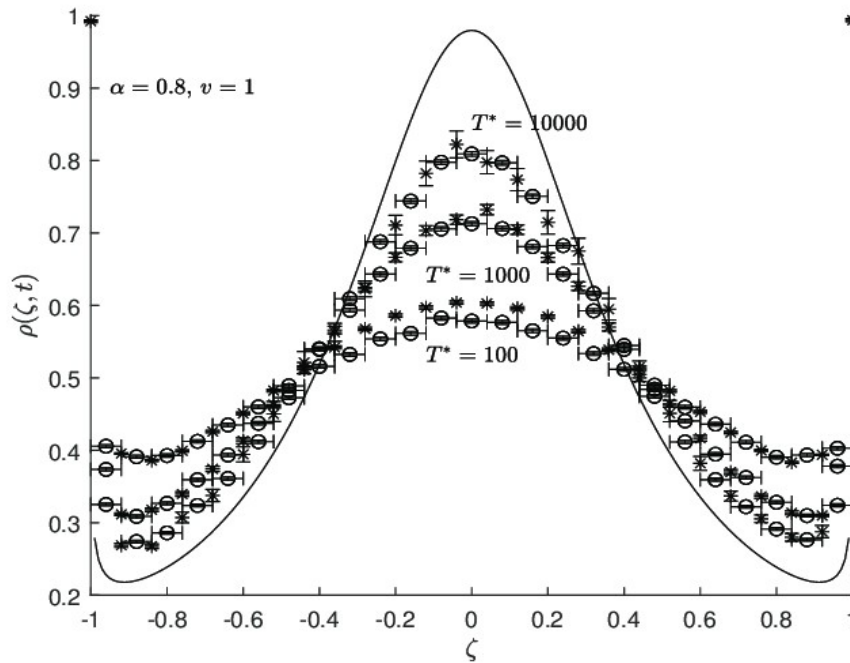


Figure 2. Плотность распределения частиц для значения  $\alpha = 0,8$  и заданных значений  $T^*$

In all considered cases, the asymptotic distribution of particles at  $t \rightarrow \infty$  and  $x \rightarrow \infty$  is described by equations of the same type. The difference between these equations is only in the order of the derivative with respect to time or coordinate and in the diffusion coefficient.

#### IV.CONCLUSION

- Study of the regularities of the influence of diffusion and mass transfer in capillary-porous bodies.
- A promising approach to providing a microclimate in buildings is to create conditions for the implementation of energy-efficient mass transfer processes through external building envelopes.
- The use of the theory of anomalous diffusion is at the initial stage of research.
- The anomalous diffusion model is based on the continuous-time random walk model (CTRW), which describes the random walk of a particle using a hop-trap mechanism.

#### REFERENCES

- [1] Saenko, V.V.; Kovalnogov, V.N.; Fedorov, R.V.; Chamchian, Y.E. Numerical Solution to Anomalous Diffusion Equations for LevyWalks. *Mathematics* 2021, 9, 3219. <https://doi.org/10.3390/math9243219>
- [2] Saenko, V.V.; Kovalnogov, V.N.; Fedorov, R.V.; Generalov, D.A.; Tsvetova, E.V. Numerical Method for Solving of the Anomalous Diffusion Equation Based on a Local Estimate of the Monte Carlo Method. *Mathematics* 2022, 10, 511. <https://doi.org/10.3390/math10030511>
- [3] Kovalnogov, V.N., Fedorov, R.V., Chamchian, Y.E. Models of Applied Mathematics in the Problems of Energy Efficiency of Buildings and Structures. *AIP Conference Proceedings* 2425, 420033 (2022); <https://doi.org/10.1063/5.0081379>
- [4] Chamchian, Y.E., Kovalnogov, V.N., Suranov, D.V. Modeling, research and development of technical properties of exterior walls and PVC windows to influence building microclimate. *AIP Conference Proceedings* 2040, 150008 (2018); <https://doi.org/10.1063/1.5079211>
- [5] Kovalnogov, V.N., Chamchian, Y.E., Suranov, D.V. Modeling, research and development of the system for optimal heat consumption of a building. *AIP Conference Proceedings* 1738, 480006 (2016); <https://doi.org/10.1063/1.4952242>
- [6] Kovalnogov, V.N., Chamchian, Y.E. Development and research of an intellectual power system for controlling microclimate in buildings. *International Journal of Energy for a Clean Environment*, 2016, 17(2-4), pp. 261–278; DOI: 10.1615/InterJenerCleanEnv.2016019207