Verification of the model for calculating conjugated heat and moisture transfer when moistening porous material

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Abstract. This paper presents a mathematical model used to calculate conjugated heat and moisture transfer in porous building materials. The initial region of the sorption isotherm for a given material was reconstructed based on the experimental data on moisture transfer in aerated concrete. The calculation results are compared with the experimental data on porous material moistening under different heat and moisture conditions. The calculations performed confirmed that model works well for sorption moistening, and not quite well with capillary impregnation. This does not exclude the possibility of engineering calculations using this model; however, at over-hygroscopic region their accuracy is not quite high.

1. Introduction
There is no single phenomenological approach to simulate numerically the processes of conjugated heat and moisture transfer in porous media as applied to the building envelope. The main difference between the calculation hygrothermal models is the choice of different moisture transfer potentials. For example, the model of [1] uses the temperature, the partial pressure of water vapor, and the air pressure as transfer potentials. For single-layer walls from a porous material, a model for calculating conjugated heat and moisture transfer, considering the moisture content gradient as the moisture transfer potential, is proposed in [2]. The calculation model of [3] takes the pressure and the temperature of capillary suction as transfer potentials. In some studies, vapor density is used as the potential for moisture transfer [4]. To create a calculation model of coupled heat and moisture transfer, Kunzel used temperature and relative humidity as transfer potentials [5]. Considering the variety of computational research, the verification of numerical solutions is the fundamental issue. To verify the models, comparison with analytical solutions [6], comparison with simulation results of other models [7], or comparison with experimental test data [8] are usually used. In this study, the model of conjugate heat and moisture transfer [5] is verified on experimental data on moistening the aerated concrete (porous building material) under various heat and humidity conditions.

2. Mathematical model
It is advisable to analyze the thermal and moisture state of the enclosures using non-stationary calculation models. Non-stationary computational models allow the most accurate prediction of alteration in the moisture and thermal characteristics of porous materials in the enclosure over time. One of the most popular non-stationary models of conjugate heat and moisture transfer is the Kunzel model [5]. In this model, the temperature and relative humidity are taken as transfer potentials.

The mathematical record of this model can be represented in the form of balance equations for heat and moisture transfer:
\[ \frac{\partial H}{\partial T} = \nabla (\lambda \nabla T) + h \nabla (\mu \nabla (\varphi p_{\text{sat}})) \]  

(1)

\[ \frac{\partial W}{\partial \varphi} = \nabla (D_{\phi} \nabla \varphi + \mu \nabla (\varphi p_{\text{sat}})) \]  

(2)

where \( T \) is temperature (°C); \( \varphi \) is relative humidity (%); \( H \) is enthalpy of a wetted material (J/m\(^3\)), \( H = H_c + H_w \), \( H_c \) is enthalpy of a dry material, \( H_w \) is enthalpy of moisture; \( t \) is time (hour); \( \lambda \) is the coefficient of thermal conductivity of a wetted material (W/m°C); \( h \) is heat of transition from a liquid to a vapor phase (J/kg); \( D_{\phi} \) is coefficient of liquid diffusion (m\(^2\)/s); \( \mu \) is coefficient of vapor permeability of a material (kg/m·s·Pa), \( p_{\text{sat}} \) is the pressure of vapor saturation at a given temperature (Pa); \( W \) is bulk material moisture (kg/m\(^3\)).

In the right part of presented equation (1), the first term is associated with heat transfer by thermal conductivity, and the second term takes into account material cooling during liquid evaporation or heat release during vapor condensation. Equation (2) takes into account transfer of moisture in a porous material in the form of liquid and vapor flows. To solve this system of equations, boundary conditions of heat and moisture transfer of kind I or III are used.

Using the presented equations of heat and moisture transfer (1-2), a computer program for non-stationary calculations of changes in the thermal and moisture characteristics of porous materials in enclosures was developed. The system of equations was approximated by a semi-implicit difference scheme. The Fortran programming language was used in the calculation algorithm.

When solving the system of equations (1-2), we should obtain a sorption isotherm of the considered porous materials as part of the enclosure. If sorption moistening occurs at relatively low material humidity, moisture transfers in the form of vapor movement; then the following expression is valid:

\[ \frac{\partial W}{\partial \varphi} = \frac{\mu p_{\text{sat}}}{D_w} \]  

(3)

Based on this expression, the sorption isotherm, which is the dependence of derivative \( \partial W / \partial \varphi \), can be determined. The calculations are performed using the example of a porous building material: aerated concrete [9]. Based on the experimental coefficient of vapor permeability \( \mu \) and the effective coefficient of moisture diffusion \( D_w \) of aerated concrete, we have determined this dependence for the conditions of low humidity of aerated concrete. Using the obtained dependence, the initial section of the sorption isotherm of aerated concrete (the marked section of the isotherm in figure 1) was calculated. Earlier, the sorption isotherm for aerated concrete at low humidity values was determined by extrapolating the experimental data obtained at high humidity values. As a result, the sorption isotherm in the initial section had a lower slope as compared to the results obtained in this work (dashed line in figure 1).
Figure 1. Sorption isotherm for aerated concrete with the density of 600 kg/m³ at 20°C.

As it can be seen from the results presented in this figure, at low relative air humidity, a sharp increase in relative mass humidity of aerated concrete $W$ is observed. According to the common classification, the sorption isotherm obtained for aerated concrete can be defined as the isotherm of type 2. This type of isotherm is typical of materials with coarse porosity, characterized by strong interaction of the material with water.

3. Results of calculations on sorption moistening

The developed program was tested using previous experimental data on the processes of heat and moisture transfer in the samples of aerated concrete under various conditions. To do this, sorption moistening of aerated concrete was calculated at a temperature of 20°C and in the presence of a moisture gradient [9] (see figure 2). Both in calculations and in experiments, dry samples of aerated concrete under isothermal conditions were considered. The lateral surfaces of samples were heat and moisture insulated. The lower surfaces of samples were in a chamber with high air humidity, and the upper surfaces were in a chamber with a sorbent that provided almost zero air humidity. In calculations the conditions of the third kind with standard coefficients of heat and moisture transfer were assumed at the boundaries of samples, taking into account a decrease in the coefficients of moisture transfer due to the presence of an air layer between the sample and the water surface.

Experimental data (symbols) and the results of calculations (lines) on moisture distribution in the samples of aerated concrete at different points in time are presented in figure 2.
Figure 2. Calculation results (lines) and experimental data (symbols) on sorption humidification of aerated concrete at 20°C.

The calculation results and experimental data agree in figure 2. In addition, according to figure 2, a displacement of the boundary of material moistening zone was observed along the sample height, and this is associated with the steep initial section of the sorption isotherm, noted previously. The dashed line in figure 2 displays the results of calculations if the sorption isotherm for aerated concrete does not take into account a sharp increase in humidity in the initial section, as it is proposed in [5]. We can see that in this case the calculation describes the experimental results worse, especially at the initial moments.

The dependence of the coefficient of liquid moisture diffusion was determined by approximating the experimental dependence of the effective coefficient of moisture diffusion on humidity taking into account the sorption isotherm and the vapor permeability coefficient of aerated concrete. In the sorption range this dependence has the following form:

$$\log(D_\varphi) = 14,492 \varphi - 19,047.$$  \hspace{1cm} (4)

At the next stage of research, to verify the computational model, sorption moistening of aerated concrete was calculated at a higher temperature in the presence of a moisture gradient. The side surfaces of aerated concrete samples were insulated from heat and moisture. The lower surfaces of samples were located in a container with air at a temperature of 65°C and humidity of about 100%, and the upper surfaces were placed in a container with air at a temperature of 71°C and humidity of about 10%. The upper surfaces of samples were moisture-proof.

The results of comparing the experimental and calculation data are presented in figure 3. It can be seen that the results of calculations and experiments agree. According to calculations, more moisture accumulated in the samples with moisture-proof upper surfaces as compared to the samples with not-insulated upper surfaces.
Data in figure 3 show that the moisture content of the material in the lower part of samples is higher than 11 ÷ 13%. According to the previously obtained sorption isotherm (figure 1), this corresponds to relative air humidity close to 90%. At higher humidity values, a liquid flow will be added to the flow of moisture in the form of vapor. Thus, with a further increase in the content of moisture in the material, the calculations should also consider the diffusion of liquid moisture.

4. Results of calculations on capillary moistening
At the next stage of work, to verify the calculation model of unsteady heat and moisture transfer, capillary moistening of aerated concrete at a temperature of 20°C was calculated [9]. At that, the lower surface of aerated concrete samples contacted with water. In this case, \( \varphi = 100\% \), it was assumed that the moisture content of material equaled the limiting moisture saturation, and at relative humidity of up to 90%, the relation between air and material humidity coincided with the sorption isotherm. The highest moisture saturation for aerated concrete with a density of 600 kg/m\(^3\) was determined experimentally; it was equal to 340 kg/m\(^3\).

At capillary impregnation, the dependence of the coefficient of liquid moisture diffusion was determined using the approximation of the experimental dependence of the effective coefficient of moisture diffusion on humidity, taking into account the sorption isotherm of aerated concrete:

\[
\log(D,\varphi) = 22.8\varphi - 26
\]  

(5)

Figure 3. Data of calculations (lines) and experiments (symbols) on sorption moistening of aerated concrete at 65°C: 1 - with moisture-insulated upper ends; 2 - without moisture-insulated upper ends.

Figure 4. The calculation results and experimental data obtained for capillary impregnation of aerated concrete at 20°C.
The satisfactory agreement between the calculation results and experimental data for capillary moistening of aerated concrete can be seen in Figure 2. It can be also noted that at capillary impregnation, moisture accumulation is more significant and intense in aerated concrete than that at sorption moistening.

5. Conclusions
As the comparisons of calculation and experimental results show, the considered model of unsteady heat and moisture transfer can be used to describe sorption moistening of porous building materials. We can see satisfactory agreement between calculations and experiments when using capillary impregnation. This does not exclude the possibility of engineering calculations using this model; however, in the superhygroscopic region, their accuracy will not be very high.

The advantages of the considered model of conjugate heat and moisture transfer include relatively small number of required transfer coefficients and continuity of transfer potentials at the boundaries between different materials. This simplifies the calculations applied to multi-layer enclosures greatly.

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