EMPIRICAL FORMULAS FOR SORPTION ISOTHERMS OF MATERIALS OBTAINED BASED ON WOOD WASTE

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Annotation. The article proposes empirical formulas that are more accurate for the analytical expression of the sorption isotherms of some building materials obtained from wood waste used in the external enclosing structures of buildings.

Key words: Humidity regime, sorption humidity, sorption isotherm, regression equation, regression coefficient, correlation attitude, adequacy.

Аннотация. В статье предлагаются эмпирические формулы, более точные для аналитического выражения изотерм сорбции некоторых строительных материалов, полученных на основе древесных отходов, применяемых в наружных ограждающих конструкциях зданий.

Ключеве слова: Влажностный режим, сорбционная влажность, изотерма сорбции, уравнение регрессии, коэффициент регрессии, корреляционное отношение, адекватность.

Аннотация. Мақолада биноларнинг ташқи тўсиқ конструкцияларида қўлланиладиган ёғоч чиқиндилари асосида олинган айрим қурилиш материалларининг сорбция изотермаларини юқори аниқликда аналитик ифодалаш учун эмпирик формулалар тавсия қилинган.

Калит сўзлар: намлик режими, сорбцион намлик, сорбция изотермаси, регрессия тенгламаси, регрессия коэффициенти, корреляцион нисбат, адекватлик.

Introduction. Wood and other known building materials obtained using wood processing waste are widely used in the construction of buildings. For example, fibrolite on Portland cement and magnesia cement, arbolite on Portland cement, chipboard and wood-fiber boards, even sawdust itself are used in the construction of buildings for various purposes. Some of them are used in building structures as structural and thermal insulation material, and some as thermal insulation material. It is known that wood itself is relatively moisture-absorbing, compared to other natural materials. Construction materials obtained from wood waste also have this property.

The value of the equilibrium moisture content of the material, especially during the operation stage of the external enclosing structure, is of great importance. Equilibrium humidity depends on the sorption properties of the material, as well as the properties of the ingredient included in the material. The thermal engineering conditions and humidity conditions of enclosing structures depend on each other. An increase in the humidity of the material of any structural layer causes an increase in its thermal conductivity and, consequently, leads to a decrease in the thermal insulation qualities of the enclosing structure. An unfavorable thermal regime, in turn, has a significant impact on the humidity regime in the structure. Builders and designers are most interested in the moisture state of structural layers during the operation of buildings. It primarily depends on the sorption properties of the materials used in the design. Therefore, when designing building enclosing structures, it is necessary to take into account the sorption characteristics of the materials used.

Review of literature and methodology. For all known building materials of natural and artificial origin, the dependence of the value of sorption moisture on the relative humidity of the air has been experimentally determined. These dependencies are usually given in tabular form in normative and reference literature. [1], [2], [3]. These data are given for an air temperature of about t=20 ^{o}C. Assuming that the relative air humidity in the thickness of the structures does not drop below 40%, the experimental values of the sorption moisture content of materials are given for values of relative air humidity within the range of $\varphi \epsilon 40...100\%$.

Scientists have developed calculation methods for predicting the moisture state in the enclosing structure of a building, taking into account external and internal operating conditions [3], [4], [5]. Based on such theoretical works, the "Guide to Calculating the Humidity Regime of Building Enclosing Structures" (Руководство по расчету влажностного режима ограждающих конструкций зданий) has been developed for practical assistance to specialists. [1]. In such calculations, performers are forced to use discrete values of the sorption moisture content of the material, determined for specific (usually 40, 60, 80, 90, 97%) values of relative air humidity. For intermediate values of relative air humidity, the value of sorption humidity is determined by interpolation. In this case, in the calculations of the humidity regime of the enclosing structure, some error occurs in determining the sorption humidity of the material, especially in the curvilinear sections of the sorption isotherm.

In calculations of the humidity regime of enclosing structures for the purpose of determining operational humidity, it is advisable to use analytical expressions for the dependence of the sorption humidity of the material on the relative humidity of the air, especially when performing the calculation using computer technologies.

It should be noted that a mathematical description of the sorption process has not yet been developed that would allow the determination of the sorption moisture content of various materials by analytical means without conducting special long-term laboratory experiments. However, calculations of the sorption moisture content of building materials are known using empirical equations of the sorption isotherm obtained on the basis of experimental data. Let's look at some of them.

L.B. Zimmermanis [6] attempted to theoretically substantiate the sorption isotherm equation in the form:

$$W_c = [W_{0^\circ} - \alpha_m \cdot (T - 273)] \cdot \varphi \cdot a_o \cdot K^{\varphi}, \quad (1)$$

где W_{0° - equilibrium sorption humidity at 0°C;

α_m - thermal coefficient of limiting sorption;

a_o - material structural sorption activity;

К - coefficient of increase in sorption activity;

φ - relative air humidity.

As a result of processing a large amount of experimental material on the study of sorption isotherms, he managed to compile a table of empirical coefficients of equation (1), applicable to aerated concrete with a density of 300, 400, 600, 800, and 1000 kg/m^3, to structural foam concrete with a density of 800, 900, and 1000 kg/m^3, as well as to heat-insulating foam concrete with a density of 300, 400, 500, 600, and 700 kg/m^3.

Academician A.V. Lykov [7] proposed to describe the sorption isotherm by an empirical equation

$$W_c = \frac{a \cdot \varphi}{b - \varphi}, \quad (2) \quad \text{at} \quad \varphi \in (0{,}1 \div 0{,}9),$$

where *a* and *b* - are empirical coefficients that depend on the temperature of the environment and

the differentiated porosity of the material.

L.M. Miniovich [8], as a result of studying the sorption moisture of various materials, came to the conclusion that the sorption isotherm can be described by the equation

$$\lg W_c = A \cdot \varphi + \lg(B + C \cdot T) \quad (3) \quad \text{at} \quad \varphi \in (0{,}1 \div 0{,}9),$$

where A, B and C – empirical coefficients.

A.U. Franchuk [9] proposed calculating the equilibrium sorption moisture content of materials using the empirical equation

$$W_c = \frac{\varphi^2 + s}{p}, \quad (4)$$

where S, P – sorption coefficients, depending on the properties of the material and temperature.

Kachura [10] suggests describing experimental sorption isotherms using an equation of the form

$$W_c = \frac{1}{a - b \cdot \varphi}, \quad (5)$$

He also determined the values of the empirical coefficients a and b for aerated concrete with a density of 650 kg/m3 at an ambient temperature of +20 °C: a = 1.876; b = 0.18.

Unfortunately, the average error of approximation of experimental isotherms of materials, estimated by the formula

$$\varepsilon_{av} = \frac{1}{n} \cdot \sum \left| \frac{W_e - W_c}{W_c} \right| \cdot 100\ \%, \quad (6)$$

for all the equations considered above is more 22 % [10].

In this article, for the analytical expression of the dependence of the sorption humidity ω of various materials on the relative air humidity φ, the author proposes an empirical formula of the following type

$$W_c = \frac{a + b \cdot \varphi}{1 - c \cdot \varphi}. \quad (7)$$

Here the values of relative air humidity are taken as fractions of 1. The values of *c* in the transformation function (1–c·φ) are within the range of 0,5 and 1, and for different materials are determined by an iterative method using multi-step regression analysis. After transforming the experimental values of sorption humidity, the coefficients *a* and *b* of equation (7) are determined by the least squares method. When choosing a value *c* with the main criterion, the minimum residual dispersion between the experimental values of sorption moisture *W*e and the calculated values *W*c, determined using the empirical formula (7), is adopted. The relative error at an experimental point is determined by the formula

$$\varepsilon_i = \frac{W_e - W_c}{W_c} \cdot 100\%. \quad (8)$$

To check the adequacy of the equation, the calculated value of the Fisher criterion is determined by the formula [11]

$$F_c = \frac{S_w^2}{S_o^2}, \quad (9)$$

where s_w^2 - is the dispersion of experimental values of sorption humidity relative to its average,

is determined by the formula [11]

$$s_w^2 = \frac{1}{n-1}\left[\sum_{i=1}^{n} W_i^2 - \left(\sum_{i=1}^{n} W_i\right)^2 / n\right]; \quad (10)$$

where *n* - total number of determined values of sorption humidity;

W$_i$ - sorption moisture content of the material at the experimental points of the sorption

isotherm, %;

s_o^2 - residual dispersion between the experimental values of sorption moisture and the

calculated values; it is determined by the formula [11]

$$s_o^2 = \frac{1}{n-k}\sum_{i=1}^{n}\left(W_e - W_c\right)^2 , \qquad (11)$$

where W_c - calculated values of sorption moisture content of the material, %, determined by formula (7);

k=2 - number of unknown coefficients in equation (7).

The tabular value of the Fisher criterion is determined in accordance with the degrees of freedom of the variances (n-1=6) and (n-k=5). If the condition $F_c > F_t$ is met, the equation recommended for describing the sorption isotherm is considered adequate [11]. The average value of the relative approximation error is determined by formula (6). The closeness of the relationship between the sorption moisture content of the material and the relative humidity of the air is estimated by the value of the correlation ratio, determined by the formula [11]

$$\eta = \sqrt{1 - \frac{S_o^2}{S_w^2}}., \qquad (12)$$

For values of the correlation ratio ŋ close to 1, the correlation between the sorption moisture content of the material *W* and the relative air humidity φ is considered very strong.

Results. The unknown coefficients of the sorption equation (7) for arbolite with a density of 600 kg/m3 were determined on the basis of experimental data given in [1]. In Table 1 shows the results of calculations of residual dispersions and the corresponding values of the parameter c and the coefficients *a* and *b* for arbolite.

Table 1

Material	Para-meters	Meanings					Regression coefficients	
							a	***b***
Arbolite γ_o=600 kg/m^3	***c***	0,7	0,705	**0,71**	0,715	0,72	2,53244	3,29057
	S_o^2	0,0380	0,0362	**0,0359**	0,0371	0,04		

As can be seen from Table 1, for arbolite with a density of γ_o=600 kg/m^3, the minimum value of residual dispersion corresponds to the desired parameter *c*=0,71 and regression coefficients *a*=2,53244 and *b*=3,29057. Thus, for arbolite with a density of γ_o=600 kg/m^3, the sorption isotherm can be expressed by the following empirical equation

$$W_c = \frac{2{,}53244 + 3{,}29057 \cdot \varphi}{1 - 0{,}71 \cdot \varphi} . \qquad (13)$$

The results of checking the adequacy of this equation are shown in Table 2. The calculated value of the Fisher criterion, determined by formula (9), corresponding to the minimum value of the residual variance, is F_c=772. The tabular value of the Fisher criterion, corresponding to the degrees of freedom of the variances S_w^2 (n-1=6) and S_o^2 (n-k=5), is equal to F_t=4,95 [11]. Since F_c=773>F_t=4.95, regression equation (13), for describing the sorption isotherm of wood concrete γ_o=600 kg/m3, can be considered adequate. The average relative approximation error calculated using formula (6) is only ε_{av}=1,38%. The value of the correlation ratio, determined by formula (12), is equal to ŋ=0.999, which indicates the presence of a very strong correlation between the sorption moisture of arbolite and the relative humidity of the air.

Table 2. Statistical data for arbolite γ_o=600 kg/m^3 at c=0,71

№	φ	We	Wc	W_e- W_c	ε_i, %	ε_{av}, %	S_w^2	F_c	F_t
1	0,4	5,5	5,37	0,13	2,32	1,38	27,7561	773	4,95
2	0,5	6,5	6,47	0,03	0,35				
3	0,6	7,6	7,85	-0,15	-3,20				
4	0,7	9,5	9,61	-0,11	-1,18				
5	0,8	12,0	11,95	0,05	0,36				
6	0,9	15,5	15,21	0,29	1,84				
7	1	20,0	20,08	-0,08	-0,39				

The experimental values and the graph of the calculated dependence of the sorption moisture of arbolite γ_o=600 kg/m^3 on the relative air humidity are shown in Fig. 1.

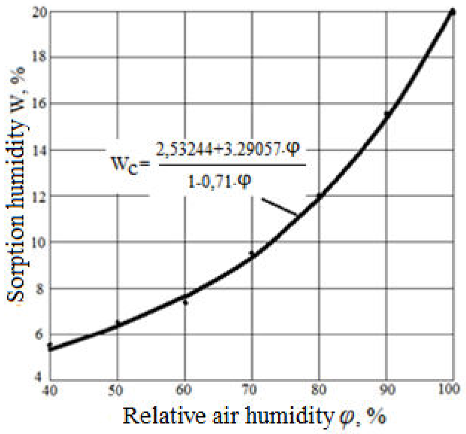

Fig. 1. Sorption isotherm of arbolite with density γo =600 kg/m3: • - experimental values of sorption humidity [1].

For a fibrolite made of Portland cement with a density of γ_o=400 kg/m3, the coefficients of the sorption equation (7) were similarly determined based on the experimental data given in [1]. In Table 3 shows the results of calculating the residual variances S_o^2 and the corresponding values of the parameter *c* and the coefficients *a* and *b* for the slab.

Table 3

Material	Para-meters	Meanings					Regression coefficients	
							a	***b***
Fibrolite slab on Portland cement γ_o=400 kg/m^3	*c*	0,895	0,9	**0,905**	0,91	0,915	3,5238	- 0,9978
	S_o^2	0,3314	0,2697	**0,2594**	0,3176	0,4677		

As can be seen from Table 3, for a fibrolite slab on Portland cement with a density γ_o=400 kg/m^3, the minimum value of the residual dispersion corresponds to the desired parameter *c*=0,905 and regression coefficients *a*=3,5238 and *b*= - 0,9978. Thus, for this material the sorption isotherm can be expressed by the following empirical equation

$$W_c = \frac{3{,}5238 - 0{,}9957\cdot\varphi}{1 - 0{,}905\cdot\varphi}\ . \qquad (14)$$

The results of checking the adequacy of this equation are given in Table 4. The calculated value of the Fisher criterion, determined by formula (9), corresponding to the minimum value of the residual variance, is equal to F_c=229. The tabular value of the Fisher criterion corresponding to the degrees of freedom of variances S_w^2 (n-1=6) and S_o^2 (n-k=5) is F_t=4,95 [11]. Since Fc=229>Ft=4,95, the regression equation (14) can be considered adequate to describe the sorption isotherm of the fibrolite slab γ_o=400 kg/m^3. The average relative approximation error calculated using formula (6) is ε_{av}=3,45%. The value of the correlation ratio, determined by formula (12), is ŋ=0.997, which indicates the presence of a very strong correlation between the sorption moisture content of fibrolite on Portland cement and the relative humidity of the air.

Table 4. Statistical data for fibrolite slab on Portland cement γ_0=400 kg/m^3 at c=0,905

№	φ	We	Wc	W_e- W_c	ε_i, %	ε_{av}, %	S_w^2	F_c	F_t
1	0,4	4,8	4,89	-0,09	-2,01	3,45	59,5361	229	4,95
2	0,5	5,7	5,52	0,18	3,13				
3	0,6	6,6	6,41	0,19	3,07				
4	0,7	7,5	7,71	-0,21	-2,76				
5	0,8	9,2	9,88	-0,68	-6,89				
6	0,9	15,0	14,16	0,84	5,89				
7	1	26,5	26,61	-0,11	-2,41				

Experimental values and a graph of the calculated dependence of the sorption humidity of fibrolite slab on Portland cement γ_o =400 kg/m^3 on relative air humidity are shown in Fig. 2.

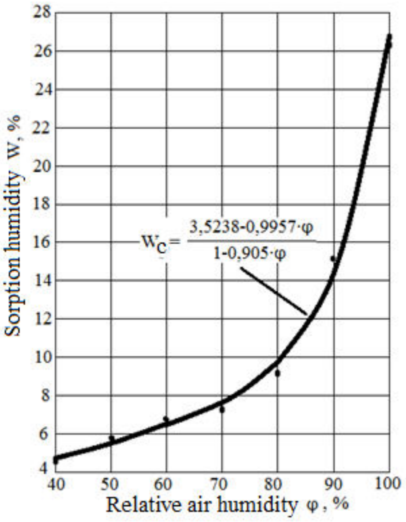

Fig. 2. Isotherm of sorption of fibrolite slab on Portland cement with density γo =400 kg/m3:

• - experimental values of sorption humidity [1].

For a fibrolite slab on magnesia cement with a density of 335 kg/m3, the coefficients of the sorption equation (7) were determined based on the experimental data given in [3]. In Table 5 shows the results of calculating the residual variances S_o^2 and the corresponding values of the parameter *c* and the coefficients *a* and *b* for the slab.

Table 5

Material	Para-meters	Meanings					Regression coefficients	
							a	***b***
Fibrolite slab on magnesia cement $\gamma_\circ$=335 kg/m^3	***c***	0,974	0,975	**0,976**	0,977	0,978	6,27467	- 3,01
	S_o^2	6,80	4,3516	**4,0239**	6,4097	12,257		

As can be seen from Table 5, for a fibrolite slab on magnesia cement with a density of γ_o=335 kg/m3, the minimum value of the residual dispersion corresponds to the desired parameter *c*=0,976 and the regression coefficients *a*=6,27467 and *b*= -3,01. Thus, for this material the sorption isotherm can be expressed by the following empirical equation

$$W_c = \frac{6,27467 - 3,01\cdot\varphi}{1 - 0,976\cdot\varphi} \quad . \qquad (15)$$

The results of checking the adequacy of this equation are given in Table 6. The calculated value of the Fisher criterion, determined by formula (9), corresponding to the minimum value of the residual variance, is equal to F_c=523. The tabular value of the Fisher criterion, corresponding to the degrees of freedom of variances S_w^2 (n-1=6) and S_o^2 (n-k=5), is equal to F_t=4,95 [11]. Since F_c=523>F_t=4,95, the regression equation (15) for describing the sorption isotherm of the fibrolite slab on magnesia cement γ_o=335 kg/m3 can be considered adequate. The average relative approximation error calculated using formula (6) is ε_{av}=6,12%. The value of the correlation ratio, determined by formula (12), is ŋ=0.998, which indicates the presence of a very strong correlation between the sorption moisture content of the fibrolite slab on magnesia cement and the relative humidity of the air.

Table 6. Statistical data for fibrolite slab on magnesia cement γ_o =335 kg/m^3 at c=0,976

№	φ	We	Wc	W_e- W_c	ε_i, %	ε_{av}, %	S_w^2	F_c	F_t
1	0,4	7,7	8,31	-0,61	-7,43	6,12	2104,5557	523	4,95
2	0,5	9,4	9,31	0,09	0,9				
3	0,6	11,4	10,78	0,62	5,71				
4	0,7	14,2	13,15	1,05	7,93				
5	0,8	18,8	17,64	1,16	6,57				
6	0,9	25,4	29,32	-3,92	-13,38				
7	1	134,8	136,03	-1,23	-0,91				

The experimental values and the graph of the calculated dependence of the sorption humidityof fibrolite on magnesia cement γ_o =335 kg/m3 on the relative air humidity are shown in Fig. 3.

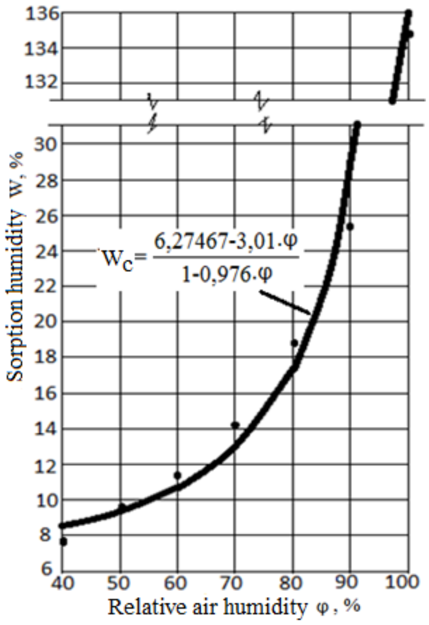

Fig. 3. Isotherm of sorption of fibrolite on magnesia cement with density γo=335 kg/m3: • - experimental values of sorption humidity [3].

After some processing, wood sawdust can be used as insulation in building coverings. For sawdust with a density of $\gamma_{\circ}$=120 kg/m^3, the coefficients of the sorption equation (7) were similarly determined based on the experimental data given in [1]. Table 7 shows the results of calculations of residual variances S_o^2 and the corresponding values of the parameter *c* and the coefficients *a* and *b* for wood sawdust.

Table 7

Material	Para-meters	Meanings					Regression coefficients	
							a	***b***
Wood sawdust $\gamma_{\circ}$=120 kg/m^3	***c***	0,895	0,9	**0,905**	0,91	0,915	3,5238	- 0,9978
	S_o^2	0,3314	0,2697	**0,2594**	0,3176	0,4677		

As can be seen from Table 7, for wood sawdust with a density of γ_o=120 kg/m^3, the minimum value of the residual dispersion corresponds to the desired parameter *c*=0,595 and the regression coefficients *a*=0,20249 and *b*=17,1025. Thus, for this material the sorption isotherm can be expressed by the following empirical equation

$$W_c = \frac{0,20249 + 17,1025 \cdot \varphi}{1 - 0,595 \cdot \varphi}. \qquad (16)$$

The results of the adequacy test of this equation are presented in Table 8. The calculated value of the Fisher criterion, determined by formula (9), corresponding to the minimum value of the residual variance, is F_c=320,5. The tabular value of the Fisher criterion, corresponding to the degrees of freedom of variances S_w^2 (n-1=6) and S_o^2 (n-k=5), is equal to F_t=4,95 [11]. Since F_c=320,5>F_t=4,95, the regression equation (16) for describing the sorption isotherm of wood sawdust γ_o=120 kg/m^3 can be considered adequate. The average relative approximation error calculated using formula (6) is ε_{av}=2.57%. The value of the correlation ratio, determined by formula (12), is ŋ=0,998, which indicates the presence of a very strong correlation between the sorption moisture content of sawdust and the relative humidity of the air.

Table 8. Statistical data for wood sawdust γ_o=120 kg/m^3 at *c*=0,595

№	φ	W_e	W_c	W_e- W_c	ε_i, %	ε_{av}, %	S_w^2	F_c	F_t
1	0,4	8,7	9,24	-0,54	-5,87	2,57	149,1747	320,5	4,95
2	0,5	12,5	12,46	0,04	0,31				
3	0,6	17,4	16,27	1,13	6,92				
4	0,7	21,0	20,86	0,14	0,65				
5	0,8	26,0	26,49	-0,49	-1,87				
6	0,9	33,0	33,57	-0,57	-1,7				
7	1	43,0	42,72	0,28	0,63				

The experimental values and the graph of the calculated dependence of the sorption humidity content of wood sawdust γ_o=120 kg/m^3 on the relative air humidity are shown in Fig. 4.

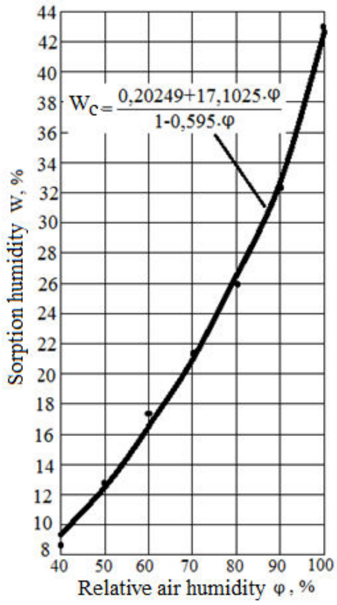

Fig. 4. Sorption isotherm of wood sawdust with density γo=120 kg/m3:

• - experimental values of sorption moisture [1].

Conclusions. From the results of the regression analysis it is evident that for materials obtained on the basis of wood waste, the dependence of the sorption moisture W on the relative air humidity φ in the range from 40 to 100% can be expressed using equations (13), (14), (15) and (16) and used in calculations of the humidity regime of enclosing structures made using the specified materials, operated in non-stationary temperature and humidity conditions.

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