

METHOD OF PREDICTION OF THERMAL CONDUCTIVITY COEFFICIENT OF WALL MATERIALS CONTAINING SALTS

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Abstract. The salt presence in porous structure of wall materials causes changes in thermal conductivity. The real value of material thermal conductivity in service conditions is necessary for engineering applications. The method of prediction of the thermal conductivity coefficient for wall materials containing salt using corrective factor is presented in the paper. By means of corrective coefficients, for well-known content of moisture and salt in wall material, it is possible to calculate thermal conductivity coefficient with regard to the presence of specific salt or mix of salts in material. The corrective coefficient values were determined for different groups of salts. The partition of salts into groups was made by means of cluster analysis, in dependence on their influence on material thermal conductivity. Clustering, in data mining, is a useful tool for discovering groups and identifying interesting distributions in the underlying data.

Keywords: thermal conductivity coefficient, wall material, salt penetration, moisture, cluster analysis, data reduction, feature extraction.

1. Introduction

The accumulation of hygroscopic water soluble salts very often takes place in capillary-porous materials of external walls of buildings in industrial plants producing salts (Ahl 2003; Lubelli *et al.* 2004; Rørig-Dalgaard 2009). Because of their good solubility, not only do salts penetrate surface layers, but also they penetrate deeper and as a result they evenly lie down on the thickness of the wall. During seasonal variations in moisture content in wall material, the crystals of anhydrous or hydrated salts form salt-solutions (van Hees and Brocken 2004; Espinosa *et al.* 2008).

Newly formed salt crystals are characterized by the thermal conductivity several times exceeding thermal conductivity of the basic material and about ten times – the conductivity of the substance (the water vapour) in pores of not salted material. Thereby, the salination of porous structure causes changes in the thermal conductivity coefficient (λ) of wall material (Koniarczyk and Gawin 2008). The assurance of the exploitive reliability of building external walls, in such conditions, demands the regard of real values of thermal conductivity coefficient in engineering calculations for material containing salt (Söylemez 1999).

The physical and statistical approach to the estimation of value of thermal conductivity coefficient of ceramic brick containing different salts (44 sorts of salt were considered) is presented in the paper. The analysis was carried out for the moisture contents and salt contents in wall material, occurring in the real service conditions of walls influenced by salts in industrial buildings.

2. Method of determination of thermal conductivity coefficient of wall material containing salt

The experimental investigation of the saline material is associated with uncontrolled migration of salt solutions and changes in physical state of salt during the preparation and tests, which lead to inaccurate results (Terheiden 2008). Since the experimental approach to test of material containing salts is rather of limited transferability, there is an urgent need for reliable calculations applicable in building practice.

The mathematical modeling (Künzel and Kiessl 1996; Nikitin and Lapko 2006; Wang *et al.* 2006) is an effective method for assessment the character as well as the intensity of salt influence on the thermal conductivity coefficient of wall materials. The mathematical model was elaborated based on the formulas of Missenard (1985) and Dulniev and Zarichniak (1974) for generalized conductivity calculation. The following factors affecting thermal conductivity coefficient of wall material with salt, were considered during calculation:

- **physical characteristics of wall material:** density, porosity, thermal conductivity coefficient of basic material, water sorptivity;
- **physicochemical characteristics of initial crystalline salt:** density, thermal conductivity coefficient of salt crystals, salt's solubility and hygroscopicity;
- **physicochemical characteristics of salt solutions,** forming in pores of material in presence of moisture: density, thermal conductivity coefficient, concentration, pressure of water vapour

above the surface of saturated solution as well as above dilute solution, hygroscopicity and heat of vaporization;

- **physicochemical characteristics of vapour**, contained in the pores of saline material: thermal conductivity coefficient of dry air, thermal conductivity coefficient of vapour considering the diffusion of water vapour;
- **salt content and moisture content** in wall material.

The validation of a calculation model requires reliable experimental investigations with well determined initial and boundary conditions, as well as accurate material properties and measurements results. For validation the calculation results of the thermal conductivity coefficient for ceramic brick were compared with the experimental measurements. The test of moisture influence on thermal conductivity was carried out for common brick without salt. The ceramic brick tested was characterized by density of 1800 kg/m³, porosity of 32% and thermal conductivity of solid part of brick 2.326 W/(mK). The comparison of calculated and experimentally determined thermal conductivity coefficient of brick for various moisture content was presented in Fig. 1.

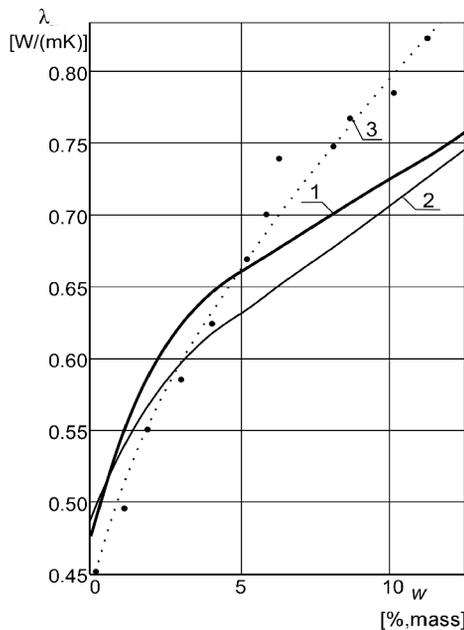


Fig. 1. Thermal conductivity coefficient of ceramic brick λ vs. moisture content w , % (by mass): 1 – calculated according to model; 2 – calculated according to Missenard (1985); 3 – experimentally determined

The experimental verification of the calculation results showed the sufficient agreement for real moisture content in practical conditions.

As a result of the first stage of coefficient λ calculation for wall material, carried out considering six selected sorts of salt of specific properties, the significant effect of salts on the increase in thermal conductivity of wall materials was found. The example of computational test results of thermal conductivity coefficient for brick in relation to moisture content as well as KCl salt content were presented in Fig. 2.

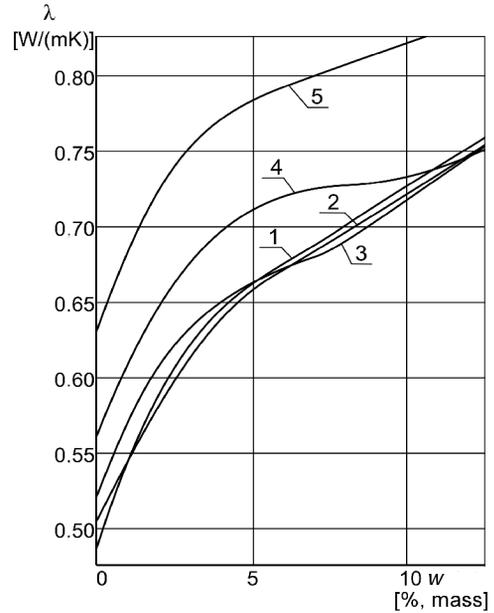


Fig. 2. Thermal conductivity coefficient of ceramic brick, density of 1800 kg/m³ in relation to moisture content w , % (by mass) and salt KCl content c , % (by mass): 1 – $c = 0$; 2 – $c = 1\%$; 3 – $c = 2\%$; 4 – $c = 4\%$; 5 – $c = 8\%$

However, for moist material the salt influence is complex and ambiguous, it means both effects were observed for coefficient λ – the increase as well as the decrease in its value (Ginevičius *et al.* 2008; Pupeikis *et al.* 2010). Based on the test results the statistic relation was obtained between coefficient λ of wall material and moisture (ω) and salt content (c), which makes it possible to calculate the thermal conductivity coefficient of wall material taking into account the phase composition of substance in material pores (see Eqs (1) and (2)):

$$\lambda = \lambda_0 + \beta\omega, \tag{1}$$

$$\lambda = \lambda_0 + \beta\omega + \gamma(c - \xi\omega), \tag{2}$$

where: λ_0 – thermal conductivity coefficient for dry material, W/(m·K); β – coefficient of the conductivity growth for 1% (by mass) increase in moisture content; γ – coefficient of the conductivity growth for 1% (by mass) increase in salt content; ξ – coefficient of shift of initial value of salinity for 1% (by mass) increase in moisture content.

It should be pointed out that the proposed Eq. (1) has very restricted application. For every wall material and sort of salt, the values of β , γ and ξ , in Eqs (1) and (2), have to be determined in special tests.

In further research on the basis of the computational experiment the considerable number of discreet values of λ coefficient for brick was obtained (3520 values), corresponding to different combinations of variability levels of examined factors for 44 different salts soluble in water. The description of the experiment performed was presented by Ezerskiy and Elcischeva (2001).

The practical application of received results demands a different approach, generalizing data from calculations of thermal conductivity coefficient as well as

making it possible to estimate qualitatively the salt influence on λ coefficient, but groups of salts rather than individual ones.

3. Cluster analysis of thermal conductivity coefficient value for wall material containing salts

Considering the number of sorts of salt found in industrial environment, the effects of salt influence on the thermal conductivity coefficient of wall material should be taken into account by use of corrective coefficients, defined for each group of salts. By means of corrective coefficients, for well-known content of moisture and salt in wall material, it is possible to calculate thermal conductivity coefficient with regard to the presence of specific salt or mix of salts in material.

In the real situation, for building walls, in which the salt accumulated, the physicochemical characteristics of salt crystals and salt solutions becomes stable (Gonçalves *et al.* 2006; Alawadhi 2008). Thus, the influence of factors such as sort of salt, salt content in material and moisture content should be considered while analysing the thermal conductivity coefficient of wall material containing salt.

The analysis of λ coefficient values for different «material + salt» systems was carried out taking into account three factors mentioned above. The possible λ values were depicted in the coordinate system and some values were arranged sufficiently close to each other, forming groups.

The method of cluster analysis was used to make the correct partition of the large set of thermal conductivity coefficient values into a smaller number of groups. The cluster analysis is one of the exact mathematical methods and it is one of the fields of the multidimensional analysis. Cluster techniques are an important tool for data analysis, data reduction and feature extraction in different applications (Anderberg 1973; Backer 1995).

The analysis permits, using mathematical statistics methods, to separate the groups (clusters) from the certain population of elements and every group significantly differs from the neighbouring groups (Tyree and Long 1999; Marton *et al.* 2008). The closest elements (with most similar properties), represented as points in n -dimensional space, are collected into groups. From a much smaller set of these representative points, it may be easier to identify the distinct features of each cluster, or the differences between clusters. This way it is possible to distinguish the elements, the properties of which are very similar within groups, but different from the elements beyond the group. Inside every cluster, the objects which are the values of λ coefficient for brick wall are similar to each other in the feature space.

The most significant methodological problems of cluster analysis are as follows: providing appropriate similarity measure including different features and the quantitative definition of groups of objects analysed. The characteristic features of the cluster analysis, distinguishing it from other methods of the solution of classification problems are as follows (Hartigan 1975):

1. Formation of clusters – non-empty subsets of objects, belonging to the initial population U .
2. The data points in clusters are collected in the way that intra-cluster similarity is maximized and inter-cluster similarity is minimized. Clusters received significantly differ apart.
3. All objects $N_j \in U$ should be classified and every object should belong to only one cluster.

The methods of cluster analysis can be broadly classified into two categories, namely hierarchical and non-hierarchical clustering. The hierarchical methods permit to merge near situated objects into separate clusters which are themselves the objects of higher level clusters. Non-hierarchical procedures of the cluster analysis, based on the distribution of the data population into separated clusters, permit to group the objects by means of separation the zones of the greatest concentration of objects in the considered space of feature. Non-hierarchical methods can be divided into parallel methods, operating simultaneously with all data population given, and iterative methods, logically operating with separated clusters (Kothari and Pitts 1999).

There are three different approaches to the problem of cluster analysis: heuristic, extreme and probabilistic. The analytical method as well as the system grouping method to carry out the cluster analysis refer to the non-hierarchical probabilistic method. The method of the system grouping was chosen for cluster analysis performing (Anderberg 1973).

By means of the system grouping method the qualitatively homogeneous population of the feature values was separated into clusters, which characterize the structure of the considered population of elements.

The feature, in the received partitioning into groups, was estimated according to the intervallic scale. The number of groups and the magnitude of intervals between them are in relation. Therefore one of the basic requirements, appearing while making a decision concerning the numbers of clusters, was the choice of such length of the interval I which would permit to divide elements of the population into groups more evenly and thus, to reach their representativity and the qualitative homogeneity.

The cluster analysis was performed according to the following algorithm:

1. Construction of the intervallic series of the value λ . The lengths of intervals I were defined according to the Sturges formula (Hartigan 1975):

$$I = (\lambda_{\max} - \lambda_{\min}) / (1 + 3.322 \lg n), \quad (3)$$

where λ_{\max} and λ_{\min} – maximum and minimum values of thermal conductivity coefficient, respectively; n – number of λ values.

2. Calculation of mean values of λ inside groups, variance S_j^2 of λ values and volume V_j of every cluster.
3. Checking the statistical significance of the difference among average λ values for clusters, according to the t-Student test.
4. Test of the homogeneity of data inside groups according to the B-Bartlett test.

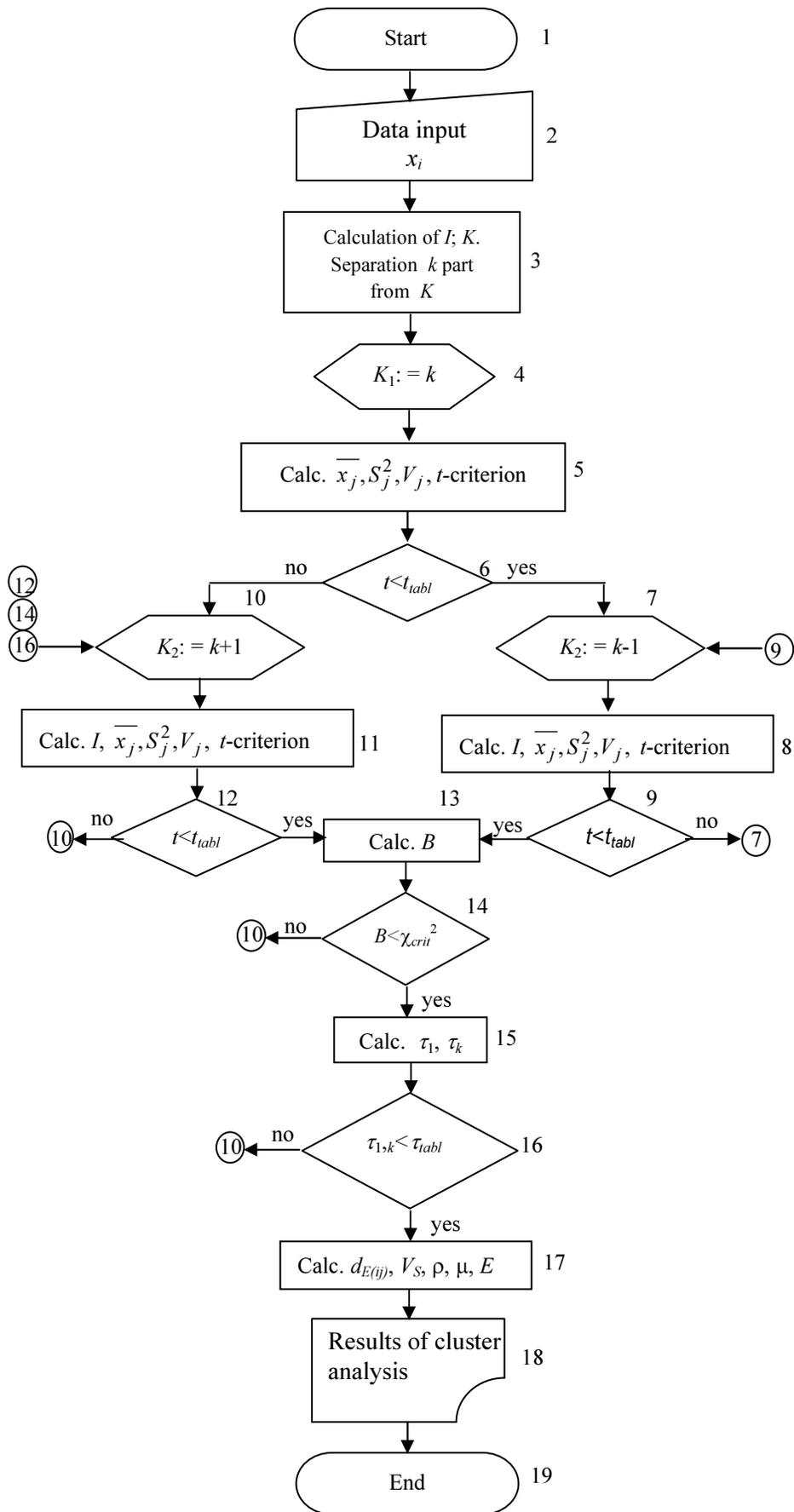


Fig. 3. Block diagram of cluster analysis algorithm

5. Checking, by means of τ -test, the first (τ_1) and last (τ_k) element of clusters (containing k values), in respect of their not accidental membership in the group.

6. Test of the similarity measure inside clusters. The Euclidean distance among data points ($d_{E(ij)}$), the coefficient of variation (V_s) and the coefficient of correlation (ρ) were calculated.

The block diagram of the algorithm of the cluster analysis was presented in Fig. 3. On the basis of diagram the computer programme in the C++ language was worked out.

Table 1. The part of salts classification and corrective coefficients ϵ , considering salt influence on thermal conductivity coefficient λ of brick wall

Salt content in material c_p , % (by mass)	Moisture content w_p , % (by mass)		
	0	1	2
	Chemical formula of salt/ corrective coefficient ϵ		
1.5	AgNO ₃ , Ba(ClO ₄) ₂ , Ba(ClO ₄) ₂ · 3H ₂ O, Ba(NO ₃) ₂ , BaF ₂ , BaS, CaBr ₂ , CaCl ₂ , CdF ₂ , CsBrO ₃ , CsCl, CsClO ₃ , KJ, LiClO ₄ , LiMnO ₄ · 3H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaBrO ₃ , NaJ, Pb(NO ₃) ₂ , RbBrO ₃ , RbNO ₃ , <u>Zn(ClO₃)₂ · 4H₂O</u> 1.026 <u>K₂SO₄, NaNO₃</u> 1.052	Ba(NO ₃) ₂ , BaF ₂ , BaS, CdF ₂ , CsBrO ₃ , CsClO ₃ , KBr, KClO ₄ , LiClO ₄ , Na ₃ PO ₄ , NaBrO ₃ , NaNO ₃ , NH ₄ Br, <u>Rb₂SO₄, RbBrO₃</u> 1.021 <u>Ba(NO₂)₂, NH₄Cl</u> 1.037	Ba(NO ₃) ₂ , BaF ₂ , BaS, CdF ₂ , CsBrO ₃ , CsClO ₃ , KClO ₄ , NH ₄ Cl, <u>RbBrO₃</u> 1.023 <u>K₂SO₄, KCl, NaCl</u> 1.036
	Ba(NO ₂) ₂ , KCl, NaCl, <u>Na₂SO₄, NaF, NH₄Cl</u> 1.068	K ₂ SO ₄ , KCl, NaCl, <u>Na₂SO₄, NaF</u> 1.051	<u>NaF</u> 1.055
3.0	AgNO ₃ , Ba(ClO ₄) ₂ , Ba(ClO ₄) ₂ · 3H ₂ O, Ba(NO ₃) ₂ , BaF ₂ , BaS, CaBr ₂ , CaCl ₂ , CdF ₂ , CoJ ₂ , CsBrO ₃ , CsCl, CsClO ₃ , KJ, LiClO ₄ , LiJ, LiMnO ₄ · 3H ₂ O, Mg(BrO ₃) ₂ · 6H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaBrO ₃ , NaJ, NaJO ₄ , Pb(NO ₃) ₂ , RbBrO ₃ , RbNO ₃ , <u>Zn(ClO₃)₂ · 4H₂O</u> 1.050 <u>K₂SO₄, NaNO₃</u> 1.105	AgNO ₃ , Ba(ClO ₄) ₂ , Ba(ClO ₄) ₂ · 3H ₂ O, CaBr ₂ , CaCl ₂ , CaJ ₂ , CsCl, KJ, LiJ, LiMnO ₄ · 3H ₂ O, Mg(BrO ₃) ₂ · 6H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaJ, NaJO ₄ , Pb(NO ₃) ₂ , <u>RbJ, RbNO₃</u> 1.023 <u>KBr, KClO₄, NaNO₃</u> 1.060 <u>Ba(NO₂)₂, K₂SO₄, NH₄Cl</u> 1.095 <u>KCl, NaCl, Na₂SO₄, NaF</u> 1.119	Ba(NO ₃) ₂ , BaF ₂ , BaS, CdF ₂ , CsBrO ₃ , CsClO ₃ , KBr, LiCl, LiClO ₄ , LiMnO ₄ · 3H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaBrO ₃ , NaJO ₄ , NaNO ₃ , NH ₄ Br, Pb(NO ₃) ₂ , Rb ₂ SO ₄ , RbBr, <u>RbCl, RbNO₃</u> 1.031 <u>K₂SO₄, KCl, NaCl, Na₂SO₄, NaF</u> 1.100
	Ba(NO ₂) ₂ , KCl, NaCl, <u>Na₂SO₄, NaF, NH₄Cl</u> 1.140		
4.5	AgNO ₃ , Ba(ClO ₄) ₂ , Ba(NO ₃) ₂ , BaS, CaBr ₂ , CaCl ₂ , CdF ₂ , CoJ ₂ , CsBrO ₃ , CsCl, CsClO ₃ , KJ, LiJ, Mg(BrO ₃) ₂ · 6H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaBrO ₃ , NaJ, NaJO ₄ , Pb(NO ₃) ₂ , <u>Zn(ClO₃)₂ · 4H₂O</u> 1.074	AgNO ₃ , Ba(ClO ₄) ₂ , Ba(NO ₃) ₂ , CaBr ₂ , CaCl ₂ , CoJ ₂ , CsCl, KJ, LiJ, Mg(BrO ₃) ₂ · 6H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaBrO ₃ , NaJ, NaJO ₄ , Pb(NO ₃) ₂ , <u>Zn(ClO₃)₂ · 4H₂O</u> 1.042	AgNO ₃ , Ba(ClO ₄) ₂ , CaBr ₂ , CaCl ₂ , CsCl, KJ, LiJ, Mg(BrO ₃) ₂ · 6H ₂ O, Mg(ClO ₄) ₂ , Na ₃ PO ₄ , NaJ, NaJO ₄ , Pb(NO ₃) ₂ , RbJ, <u>Zn(ClO₃)₂ · 4H₂O</u> 1.027
	BaF ₂ , CaJ ₂ , KClO ₄ , LiCl, LiClO ₄ , NH ₄ Br, Rb ₂ SO ₄ , RbBr, <u>RbBrO₃, RbCl, RbJ</u> 1.110 <u>KBr, NaNO₃</u> 1.144	BaF ₂ , BaS, CsBrO ₃ , CsClO ₃ , LiCl, LiClO ₄ , NH ₄ Br, Rb ₂ SO ₄ , RbBr, RbBrO ₃ , <u>RbCl, RbJ</u> 1.074 <u>KBr, KClO₄, NaNO₃</u> 1.099	Ba(NO ₃) ₂ , BaS, CdF ₂ , CsBrO ₃ , CsClO ₃ , LiCl, LiClO ₄ , NaBrO ₃ , NaNO ₃ , NH ₄ Br, Rb ₂ SO ₄ , RbBr, <u>RbBrO₃, RbCl</u> 1.062
	<u>Ba(NO₂)₂, K₂SO₄, NH₄Cl</u> 1.192 <u>KCl, NaCl, Na₂SO₄, NaF</u> 1.224	<u>Ba(NO₂)₂, K₂SO₄, NH₄Cl</u> 1.153 <u>KCl, NaCl, Na₂SO₄, NaF</u> 1.187	<u>BaF₂, KBr, KClO₄</u> 1.082 <u>Ba(NO₂)₂, K₂SO₄, Na₂SO₄, NH₄Cl</u> 1.132

4. Interpretation of cluster analysis results

On the basis of calculations the set of the feature values was obtained, which was divided into separated clusters. The suitable average value of the feature x_j was given to every separated cluster. The corrective coefficients ε , which allow regarding the material salination, were determined on the basis of the average values of the feature x_j for every cluster referred to the thermal conductivity coefficient of not salted material at the same moisture content. The results are presented in Table 1.

The thermal conductivity coefficient of the brick containing salt can be determined by means of the corrective coefficients received. The value of λ can be calculated by multiplying the thermal conductivity coefficient of not salted material of specified moisture content, for example $\lambda_{\omega 1}$, by the corrective coefficient ε_c for salt content c expected in material under service conditions:

$$\lambda_{\omega I, c} = \lambda_{\omega I} \cdot \varepsilon_c \quad (4)$$

If material contains the mix of different salts, for example, A + B + C, the corrective coefficient $\varepsilon_c^{(A+B+C)}$ is calculated as the product of corrective coefficients for individual salts $\varepsilon_c^A, \varepsilon_c^B, \varepsilon_c^C$:

$$\varepsilon_c^{(A+B+C)} = \varepsilon_c^A \cdot \varepsilon_c^B \cdot \varepsilon_c^C \quad (5)$$

5. Conclusions

The purpose of this report was to propose the way of prediction of the thermal conductivity coefficient of wall materials containing salts. The most widespread salts in the industry were classified into groups according to the degree of their influence on the thermal conductivity by means of the cluster analysis. The degree of the salt influence on the thermal conductivity of material was evaluated in consideration of the sort of salt, the salt content in wall material as well as moisture content. The corrective coefficients of thermal conductivity were determined for groups of salts.

The design value (useful for engineering applications) of thermal conductivity coefficient of brick wall containing salts can be predicted on the basis of known value of thermal conductivity coefficient of not salted material with regard of corrective coefficients, obtained. The selected values of corrective coefficients calculated are presented in the paper (Table 1).

It should be pointed out that even the best model cannot replace the real field test, because in practice there are always some effects not considered in the model. However, due to expensive and time consuming experimental investigations of the thermal behaviour of building components, calculative studies are becoming increasingly important. They are also useful for predicting the consequences of any constructive modifications or the effects of different climate conditions.

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SIENŲ DRUSKINGŲ MEDŽIAGŲ ŠILUMOS LAIDUMO KOEFICIENTO PROGNOZĖS METODAS

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Santrauka

Druskos poringųjų medžiagų sienų struktūroje sukelia jų šilumos laidumo kitimą. Tikroji eksploatacinė medžiagų šilumos laidumo koeficiento vertė būtina atliekant inžinerinius tyrimus. Straipsnyje pristatomas sienų, kurių medžiagos turi druskų, šilumos laidumo koeficiento prognozės metodas naudojant pataisos daugiklį. Naudojant pataisos koeficientus, esant tiksliai žinomam drėgmės ir druskų kiekiui sienos medžiagoje, galima apskaičiuoti šilumos laidumo koeficientą, atsižvelgus į tam tikrų druskų ar jų mišinių buvimą medžiagoje. Buvo nustatytos įvairių druskų grupių pataisos koeficientų vertės. Druskos buvo paskirstytos grupėmis pagal klasterinę analizę, priklausomai nuo jų įtakos medžiagos šilumos laidumui. Klasterių metodas yra naudinga priemonė duomenims apdoroti – grupėms atskleisti ir įdomiems duomenų pasiskirstymams rasti.

Reikšminiai žodžiai: šilumos laidumo koeficientas, sienų medžiaga, druskų įsiskverbimas, drėgmė, klasterinė analizė, duomenų redukovimas, savybių išryškėjimas.

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