Physical and chemical bases, structural and technological models of constructional thermal insulating lightweight concrete creating

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Abstract. Research object is constructional and thermal-insulating lightweight concrete (STILC) with a modified matrix in the direction improving of thermotechnical quality and durability indicators of such concrete, produced with use of porous aggregates of various petrogenesis. Motivation: the development relevance of STILC new modifications with high performance of thermotechnical quality and durability is determined by the fact that the STILC usage in the enclosing structures of buildings will significantly improve their thermal insulation function, operational reliability. Research method: the developed physical and chemical bases, structural and technological models of the modified matrix of STILC are used in researches. Research results: physical and chemical bases, structural and technological models for creating of STILC with high indicators of thermotechnical quality and weather resistance; technologies for manufacturing STILC with rational usage of technogenic formations recycling products; results of determination of thermophysical characteristics, indicators of weather resistance and other indicators of STILC operational quality. Conclusion: fundamentally new modifications of STILC with high indicators of thermal quality and weather resistance, and the main provisions of their manufacturing technology also have been developed. Based on the results of STILC samples testing, the thermophysical and mechanical properties, as well as weather resistance indicators, were determined for use in the calculations and design of enclosing structures with high thermal protection function and reliability in operation.

1. Introduction

Research object is structural thermal-insulating lightweight concrete (STILC) with a modified matrix in the direction improving of thermotechnical quality and durability indicators of such concrete, produced with use of porous aggregates of various petrogenesis. The development relevance of STILC new modifications with high performance of thermotechnical quality and durability is determined by the fact that the STILC usage in the enclosing structures of buildings will significantly improve their thermal insulation function, operational reliability and contribute to energy and resource saving [1].

The purpose of the researches is the development of physical and chemical bases, structural and technological models of STILC. Creating of STILC manufacturing technology and determining of their operational quality indicators.

The research tasks:
development of the physical and chemical bases, structural and technological models for creating of STILC with high indicators of thermotechnical quality and weather resistance;

- development of technologies for STILC manufacturing with rational usage of technogenic formations recycling products;

- determination of thermophysical characteristics, indicators of weather resistance and other indicators of STILC operational quality.

The relevance of the above research tasks is determined by the necessity to address the following main issues of resource and energy saving in construction at all its stages:

1. At the stage of production of low-energy-intensive in production, environmentally safe and cost-effective technologies for wall products and enclosing structures using ultra-lightweight thermal insulation and constructional thermal insulating concrete, manufactured with preferential use in all their components (binders and aggregates) of large-scale technogenic formations (mainly metallurgy and fuel energy industries) processing products, and characterized by high indicators of thermal quality and weather resistance.

2. At the stage of structural system elements installation and operation of residential and civil buildings – enclosing structures in prefabricated (with the use of external wall panels or wall blocks) or in a monolithic version, characterized by a high thermal protection function and reliability in operation. In connection with the above we can recommend to introduce a series of articles devoted to the problem of energy saving in all three stages of construction of buildings, published in the journal “Stroitel'nye Materialy” (“Construction Materials”) No. 6-9 [1], as well as a series of reports on organized by the Russian Academy of Sciences International conference “Technogen – 2012” in connection with 80-th anniversary of academic science of Urals inter-state issue “State and prospects of large-tonnage products of processing of technogenic wastes of metallurgy in the construction industry”. The plenary reports “Technogen-2012” are published in the journal of the Russian Academy of Sciences “Ekologia i promyshlennost Rossi” (“Ecology and Industry of Russia”) No. 10, 2012 [2].

In connection with the above we also recommend to read the following:

- publications of Saint Petersburg Polytechnic University [3] and Volgograd University of architecture and construction [4] on the problem of resource and energy saving in the construction and operation of buildings;

- publication in Proceedings of Eindhoven University of Technology (The Netherlands), Elsevier [5];

- publication of Saint-Petersburg state University of architecture and construction [6] and a patent for the invention RU2592907C1 (Bulletin of the invention No. 21 from 27.07.2016) [7] related to the manufacturing technology of non-autoclave cellular structural thermal-insulating foamed concrete that differs from conventional technology using polypropylene and basalt fiber in order to increase the bending strength under tension while reducing the required consumption of cement and, accordingly, the coefficient of thermal conductivity and shrinkage deformations.

2. Methods

For the development of technological bases of rational STILC structures creation with high indicators of thermotechnical quality the model of numerical solution of Laplace’s differential equation of thermal conductivity by means of computer realization method was created [8].

The problem of determining the thermal conductivity coefficient of STILC came down to calculating the heat flow, for which the temperature field of the concrete cell was found by solving the system of Laplace’s differential equations:

\[
\frac{\partial^2 t_{11}}{\partial x^2} + \frac{\partial^2 t_{11}}{\partial y^2} + \frac{\partial^2 t_{11}}{\partial z^2} = 0 ,
\]

\[
\frac{\partial^2 t_{12}}{\partial x^2} + \frac{\partial^2 t_{12}}{\partial y^2} + \frac{\partial^2 t_{12}}{\partial z^2} = 0 ,
\]
where $t_1$ is a function that determines the temperature field of the external component of the concrete cell (hardened cement paste or mortar); $t_2$ – function that determines the closed-loop temperature field of a concrete cell (aggregate grain).

Differential equations are solved together with conditions of temperatures ($t_1$=$t_2$) and thermal flows equality at the borders of hardened cement paste ($t_{1,x}$, $\lambda_{1}$) and aggregate ($t_{2,z}$, $\lambda_{2}$):

$$
\lambda_1 \frac{\delta t_1}{\delta x} = \lambda_2 \frac{\delta t_2}{\delta x} ;
\lambda_1 \frac{\delta t_1}{\delta x} = \lambda_2 \frac{\delta t_2}{\delta x} ;
\lambda_1 \frac{\delta t_1}{\delta z} = \lambda_2 \frac{\delta t_2}{\delta z} ;
$$

(3)

The influence of the heat flow trajectory on the thermal conductivity coefficient of a composite material is stronger, the greater is the difference in the values of heat conductivity coefficients of its components, which is illustrated in figure 1.

Figure 1. Principal diagrams of heat flows possible trajectories in a model of a lightweight concrete cell.

The numerical solution of the described calculation model makes it possible to choose the porous aggregate with the optimal structure (by the criterion of its grain thermal conductivity coefficient $\lambda_a$) when designing the STILC composition. The analysis of the determined influence of $\lambda_a/\lambda_{cp}$ ratio, where $\lambda_{cp}$ is the coefficient of hardened cement paste thermal conductivity, on the thermal conductivity of lightweight concrete (see above), shows a clear advantage in the low thermal conductivity coefficient of the structural thermal insulating expanded polystyrene concrete developed with this paper author's participation [9] in comparison with other types of lightweight concrete at equal density grade.

Thus, by analytical method with help of the developed model an expert assessment of STILC various types according to the criterion of their thermotechnical quality main indicator may be performed.

3. Results of the investigations

When developing optimal (first of all, by the criterion $\lambda_{min}$) compositions of the STILC, authors proceeded from the given below in this article physical-chemical bases provisions of obtaining the STILC with the minimum possible values of the thermal conductivity coefficient in the state of the equilibrium moisture sorption ($\omega_o$).

As the most heat-conducting component of the STILC is the hardened cement paste, the task was set to develop the low clinker composite binder (LCB) with minimum possible (at LCB activity not less than 40 MPa) indicators of thermotechnical quality ($\lambda_{min}$, $\omega_o$).

Low clinker special composite binders (LCB-S) were developed (with clinker content not more than 50 %), in which clinker was replaced by a hydraulically active component - a product of metallurgy and thermal power engineering technogenic formations processing [10].

Figure 2 shows the results of determining the optimal composition (content of cement clinker and superplasticizer C-3) of one of the main varieties of LCB-S – with the use of ground blast furnace slag.
Figure 2. Nomograph of dependence of compressive strength of hardened LCB-S cement paste (R_{28}, MPa) after 28 days of normal-humidity curing conditions, thermal conductivity coefficient in a dry state (\lambda_0, W/(m\cdot{\degree}C)) and its increment (\Delta\lambda, W/(m\cdot{\degree}C)) on 1% of humidity on the cement clinker (CC) content and the superplasticizer C-3 content at the grinding fineness of raw mixture S = 3250 cm\(^2\)/g.

It can be seen that with a decrease in the content of cement clinker to the minimum possible (up to 20%; in this case, the activity of the binder is 40 MPa), the coefficient of thermal conductivity of the binder in the dry state decreases from 0.45 W/(m\cdot{\degree}C) to 0.40 W/(m\cdot{\degree}C).

It seems that when developing low-clinker composite binders of a special class LCB-S (for STILC with high thermal quality indicators), manufactured mainly on the basis of chemically compatible technogenic waste products of their processing, it is advisable to proceed, first of all, from the following basic provisions of physical chemistry of silicates [11] and thermophysics of disperse systems [13]:

1. Improvement of thermophysical properties of LCB-S hardened cement paste is actually possible due to the inclusion in the composite binder material of such a relatively low heat conductivity and low sorption active component as a product of metallurgical slag melting processing with the forced cooling mode, which provides the amorphous phase predominant content in the granulated slag [13-16]. This refers, first of all, to non-disintegrating slags of blast furnace and ferroalloy industry.

2. In addition to actions of such favorable factors as the corresponding phase composition, lower thermal conductivity of the composite binder with hydraulically active ground metallurgical granulated slag must provide the relatively high content as the hydration products of the cryptocrystalline low-base calcium hydrosilicates type of the CSH(B), and particularly cryptocrystalline low-base hydroaluminates type of C_{2}AH_{8}.

The advantage in the relatively low thermal conductivity of cryptocrystalline structures of hardened binders, as well as structures that are mostly amorphous, can be explained by the known in the thermophysics of dispersed systems “effect of near-order phonon run” [12]. To do this authors recommend to use the following formula for the thermal conductivity coefficient \(\lambda\) of R. Peierls [18]:

\[
\lambda = 1/3 \left( l_{av} \cdot U \cdot C \right),
\]

\(l_{av}\) is average way of phonons (quasiparticles of the energy of the associated thermal oscillations of the lattice nodes of a solid body) run;

\(U\) - the speed of phonons propagation;

\(C\) – volumetric thermal capacity.
3. Contrary to the previously widespread belief that the chemical composition has insignificant influence on the thermal conductivity of building materials, it is worth noting here the results of the following studies. Thus, researches carried out at the Institute of Physical Chemistry of the Russian Academy of Sciences found that a material in the vitreous state does not finally break down to the near-range order, but only shortens to the polymeric far order, in which the structure of chains partially retains its length, despite of their curvature in 3 dimensions. Length of free run of phonons in glass in such case should depend on chemical and mineralogical composition of silicates, that, according to formula (4) should influence also on value of heat conductivity.

This is to certain extent confirmed by the results of experimental research of Zyatkova L.R., Chernyavsky I.Ya. and Miller S.N. (UralNIIStromproject) [19], who studied the thermal conductivity of semi-synthetic slag glasses of SiO$_2$-Al$_2$O$_3$-CaO-MgO system. They found out: if the density of slag glasses changes depending on their mineralogical composition quite insignificantly (from 2.54 to 2.76 t/m$^3$, i.e. only by 8.7%), then the change of their thermal conductivity is quite significant – from 0.50 to 1.50 W/m$\cdot$°C. It should be noted that the minimum values of the coefficient of thermal conductivity of slag glasses are observed on the line Al$_2$O$_3$-CaO, and the maximum values – at partial replacement of CaO and SiO$_2$ by MgO.

It is also worth noting the results of experimental researches conducted in 2007-2009 by I. I. Kuznetsova (SibADI) [20] on the influence of the relative content of the main minerals of hardened cement paste on its thermal conductivity coefficient ($\lambda_{CP}$). Indeed, the analysis of the experimental researches results showed that a relative increase in the content of alite C$_3$S leads to the increase in $\lambda_{CP}$. With a decrease in the content of C$_3$S and a corresponding increase in C$_2$S, calcium aluminate C$_3$A and calcium aluminoferrite C$_4$AF, the thermal conductivity of the hardened cement paste decreases. The content of calcium aluminate C$_3$A has the most significant effect of influence on the $\lambda_{CP}$ value.

As for the foreign experience of investigations and application of composite low clinker binders (LCB) in concrete for enclosing structures, we can note the actively progressive development of this direction in the construction industry of foreign countries. First of all, this applies to countries such as Canada, the USA [21, 22], as well as to developed countries in Western Europe [23]. This is due not only to the best thermal engineering properties of LCB in comparison with traditional cements, but also to significantly lower (up to 2 times) energy costs for their production (due to a corresponding reduction in the clinker content and, consequently, energy costs for its firing), as well as saving natural resources, in particular, limestone and reducing CO$_2$ emissions into the atmosphere during the firing of clinker [24].

4. Calculated physical model of the thermal conductivity coefficient of structural thermal insulating lightweight concrete of new modification (results of analytical studies)

To determine the efficiency of the developed LCB-S using in the structural thermal insulating concretes of new modifications (STILC-M), a principally new calculation model of the concrete thermal conductivity was developed (see figure. 3). In contrast to the previous model described above, this model is considerably closer in real structure to the STILC-M and allows significantly more accurate calculation of the thermal conductivity coefficient ($\lambda_b$) of concrete. This is determined by the fact that the new model reproduces with the highest possible accuracy the real structure of concrete: random location, size and number of filler grains in a given volume. The corresponding propagation of heat flows through the simulated sample is assumed taking into account their actual trajectories.
Figure 3. Physical model of STILC-M to the numerical determination of its thermal conductivity coefficient taking into account the aggregate granulometric composition.

The physical model of concrete is a sample in the form of a parallelepiped with a size of 80x80x75 mm (figure 3), on the space of which the coordinate grid is superimposed with a step of 1 mm. The coordinates of the nodes of the considered grid area along the X, Y, and Z axes are denoted respectively by \(i=1,2,...,80; \ j=1,2,...,80; \ k=1,2,...,75\). The lower face of the parallelepiped (at \(Z=0\)) temperature is set to \(T_{\text{low}}\), and the upper face (at \(Z=75\) mm) – to \(T_{\text{up}}\). At the same time \(T_{\text{low}}-T_{\text{up}}=1^\circ\).

The shape of the aggregate grain model is a cube with sides that are multiples of 1 mm. The size of the grain-cube face is appointed so that its volume must be equal to the volume of the aggregate grain at the actual shape, which is usually represented by a sphere.

The initial data for the development of the physical model and the subsequent calculation of the thermal conductivity coefficient \((\lambda)\) of concrete are: volume in fractions of one unit in 1 m³ of concrete aggregate minus its intergranular void; number of aggregate fractions – no more than three; volume in % of the aggregate each fraction minus the intergranular void in the total volume of the aggregate; dimensions in mm of grains of each aggregate fraction; coefficient of thermal conductivity in W/(m°C) of grains of each aggregate fraction; coefficient of thermal conductivity in W/(m°C) of hardened cement paste in concrete.

Using the given initial data, the construction of the concrete sample under study is carried out using a computer calculation based on a special program developed by the authors.

Determining of the thermal conductivity coefficient of any material is reduced to obtaining its temperature field, which is theoretically accurately described by the Laplace’s differential equation [8]:

\[
\frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2} + \frac{\partial^2 t}{\partial z^2} = 0
\]  

Equation (5) for concrete, as a non-uniform material, is solved together with the conditions of equality of temperatures and heat flows at the boundaries of the hardened cement paste and the aggregate:

\[
t_1 = t_2; \quad \lambda_1 \times \frac{\partial t_1}{\partial x} = \lambda_2 \times \frac{\partial t_2}{\partial x}; \quad \lambda_1 \times \frac{\partial t_1}{\partial y} = \lambda_2 \times \frac{\partial t_2}{\partial y}; \quad \lambda_1 \times \frac{\partial t_1}{\partial z} = \lambda_2 \times \frac{\partial t_2}{\partial z};
\]  

It was not possible to obtain by analytical way the temperature field of concrete using equation (5) with conditions (6). Therefore, the Laplace’s equation was solved using a computer by the numerical method of “dispersing residuals”.

\[
\lambda_1 \times \frac{\partial t_1}{\partial x} = \lambda_2 \times \frac{\partial t_2}{\partial x}; \quad \lambda_1 \times \frac{\partial t_1}{\partial y} = \lambda_2 \times \frac{\partial t_2}{\partial y}; \quad \lambda_1 \times \frac{\partial t_1}{\partial z} = \lambda_2 \times \frac{\partial t_2}{\partial z};
\]
The numerical interpretation of equation (5) according to the difference scheme is written as conditions (7) and (8), which are performed respectively inside homogeneous concrete materials and on the border of non-uniform ones, i.e. cement stone and aggregate:

\[ T_{i+1,j,k} + T_{i,j+1,k} + T_{i,j,k+1} + T_{i-1,j,k} + T_{i,j-1,k} + T_{i,j,k-1} - 6 \cdot T_{ijk} = 0, \quad (7) \]

where \( T \) is the temperature in the nodes of a grid; \( i, j, k \) – coordinates of nodes in figure 3.

\[ M_{x,ijk} = \lambda_x \cdot (T_{i+1,j,k} - T_{ijk}) - \lambda_x \cdot (T_{ijk} - T_{i-1,j,k}) = 0 \]
\[ M_{y,ijk} = \lambda_y \cdot (T_{i,j+1,k} - T_{ijk}) - \lambda_y \cdot (T_{ijk} - T_{i,j-1,k}) = 0 \]  
\[ M_{z,ijk} = \lambda_z \cdot (T_{ijk+1} - T_{ijk}) - \lambda_z \cdot (T_{ijk} - T_{i,j,k-1}) = 0 \]  

(8)

Here, the values \( \lambda_x \) and \( \lambda_y \) are determined by the well-known formulas of thermophysics [25] for materials with parallel and perpendicular layered structures.

The solution of the equations system (7) and (8) is carried out by the numerical method of “dispersing residuals”, the essence of which is as follows. First, an initial approximation of the temperature field is set, representing the linear change from the bottom to the top of the concrete sample faces. Next, a purposeful iteration of the grid area nodes is performed when the \( T_{ijk} \) temperature of each node changes in such a way as to minimize the sum of absolute values (or squares) of residuals in this node:

\[ H_{ijk} = |N_{ijk}| + |M_{x,ijk}| + |M_{y,ijk}| + |M_{z,ijk}| \rightarrow \text{min} \]  

(9)

After determining the temperature field using formulas (7) and (8) using the “dispersion of residuals” method on a computer, the heat flow and the coefficient of thermal conductivity of concrete are calculated using formulas (10) and (11) respectively:

\[ Q = \sum q_{ijk} = \sum \lambda_x \cdot (T_{ijk+1} - T_{ijk}) \]  
\[ \Lambda = Q/0.075, \]  

(10)  

(11)

where 0.075 is height of the accepted concrete model in meters.

Using the results of calculations on the created analytical model found the optimal structure STILC-M on the example developed by the authors modified polystyrene lightweight concrete (MPLC) [16]. Using the above-stated provisions of physical and mechanical bases of silicate materials and in particular hardened cement paste and concrete in relation to the influence of their micro and macrostructure on the thermal conductivity of such materials is established the necessity of using the components of concrete characterized by:

- optimal granulometric composition of expanded polystyrene grains, determined with help of the theoretical computations (look above formulas (5)-(11));
- the developed also by the authors low clinker composite binders [2] with the use of mechanical chemical activated modifiers [17] which provide the minimum thermal conductivity coefficient of this type concrete at a given compressive strength (\( R_c \)).

At figure 4 it is shown that the optimal structure of the MPLC is characterized by granulometric composition of expanded polystyrene grains with a 100 % content of 0-5 mm fraction.
Figure 4. The dependence of the MPLC conductivity ($\lambda_c$) on the diameter of aggregate grains (d) for given values of the aggregate grains ($\lambda_a$) coefficients of thermal conductivity, volume of aggregate minus its intergranular void of 0.6 m$^3$/m$^3$ and thermal conductivity of cement stone is 0.4 W/(m⋅°C).

5. Conclusion
Using the thermophysical bases of dispersed materials and physical and chemical bases of silicate materials, structural and technological models of constructional thermal-insulating lightweight concrete (STILC) with high indicators of thermal quality and weather resistance have been developed, taking into account the main provisions of their manufacturing technologies. It is established that the influence of the heat flow trajectory on the thermal conductivity coefficient $\lambda$ of a composite material such as STILC is the stronger the greater the difference in the values of the thermal conductivity coefficients of its components.

Based on the results of analytical studies of the heat flow trajectories influence on the thermal conductivity coefficient ($\lambda$) of STILC and its components, corresponding calculation models were constructed. Based on experimental studies of STILC optimal compositions, nomograms showing the dependence of physical and mechanical characteristics and the thermal conductivity coefficient ($\lambda$) of STILC in the dry state and its increments ($\Delta\lambda$), as well as increments of sorption humidity by 1% of the cement clinker content are constructed. In addition to the above-mentioned indicators of thermal engineering quality, weather resistance indicators were also determined for use in the calculations and design of enclosing structures characterized by a high thermal protection function.

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