Modeling the process of autoclaving treatment of cellular concrete products as control object

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Abstract. The authors consider the questions of modeling the process of autoclave treatment of cellular concrete products as a control object. The modeling method, performed in several stages, is suggested. At the first stage, a mathematical model of energy processes occurring in an autoclave, taking into account the internal heat generation during the formation of tobermorite in raw cellular concretes, is developed. The temperature dynamics of steam in an autoclave \( T_d(t) \) has been determined. At the second stage, heat transfer in a cellular concrete is modeled for a given value of \( T_d(t) \). As a result of computational experiments, the temperature dynamics \( T_m(x, y, z, t) \) in the most characteristic parts of the cellular concrete was determined. The assessment of the adequacy of the developed model was made by comparing the results of modeling with the results of experimental studies obtained with the existing process equipment.

1. Introduction
The production of cellular concrete products with specified characteristics is largely determined by the algorithms controlling the main technological processes. The strength of cellular concrete products is determined mainly by the autoclaving treatment. In this regard, the development of a mathematical model of the technological process of autoclave treatment of cellular concrete products as a control object is highly relevant.

The description of the temperature field dynamics in raw cellular concretes during their autoclave treatment under conditions of nonstationarity of parameters, by analogy with [1,2], goes down to solving a system of differential equations with partial derivatives that take into account heat and mass transfer in the autoclave environment and raw cellular concretes.

The authors of this article, understanding the complexity and lack of knowledge of the process under consideration, taking into account the fact that the dynamics of the autoclaving treatment is characterized by a vector that includes a sufficiently large number of parameters, among which there are various internal unsteady connections, and focusing on creating a mathematical model of the process under study as a control object for which a certain degree of “roughness” is permissible,
assumed it appropriate to consider the object in terms of the following assumptions and simplifications:

At the first stage it is proposed to consider raw concretes as thermally thin bodies. This allows us to create a fairly simple energy model of the dynamics of heat flows impacting the raw concretes. At the second stage, it is proposed to consider a single raw concrete example from the set loaded into the autoclave as an object with distributed parameters. The heat flux acting on the surface of this raw concrete will be determined at the first stage of modeling. As a result, at the second stage, the dynamics of thermal processes in the concrete is investigated, which allows to form an autoclave control algorithm taking into account the restrictions connected with the temperature distribution inside raw concrete. The third stage implies the use of an iterative approach to specify the dynamics of the energy model of the autoclaving process. This will allow to perform the next stage of modeling an object with distributed parameters, taking into account the refined nature of the heat flux impacting the raw concrete. This paper covers the first two stages.

The main purpose of autoclaving automation is to create conditions for a sustainable process when calcium hydroxysilicates in the form of tobermorite are formed in raw concretes, ensuring the required strength of cellular concrete products [3].

The main technological requirements for this process are:
1) Absence of air in the pores of raw concrete;
2) Complete filling of raw concrete pores with saturated steam to ensure the chemical reactions;

Technological limitations apply to:
1) the rate of heating and cooling of raw concretes;
2) the pressure in the autoclave limit value;

The control object will be understood as the combination of heating performance, physical and chemical processes occurring during the autoclave treatment of the raw cellular concrete products. The state of the object will be characterized by $X$ vector of the output coordinates, which include the temperature distribution over the product and the vapor pressure in the autoclave. We should take the steam flow rate $g_1$ supplied to the autoclave and the steam exhaust flow rate $g_2$ coming out of the autoclave as elements of $U$ vector of control action. The main perturbations are the uncertainty (within the framework of known limitations) of the physical and mineralogical composition of the raw concretes, the variation in temperature values and steam pressure supplied to the autoclave from the heat source (boiler, steam accumulator), the unsteady internal heat generation processes and heat losses to the environment through the structural elements of the autoclave.

2. Modeling Goal

Development of an adequate mathematical model of the process of autoclaving cellular concrete products with focus on its use in combination of ACS for autoclaving treatment.

The authors consider the stages of pressure increase and curing in the autoclave before which the blowing and vacuuming, necessary to form well-defined initial conditions for the raw cellular concretes and the autoclave environment, are performed.

In the autoclave, with a radius of $r_{\text{aut}}=1.35 \text{ m}$ and a length of $l_{\text{aut}}=26.5 \text{ m}$ 12 raw cellular concrete blocks of $D400$ density grade with the total mass $m_{\text{bl}}=24 \times 10^3 \text{ kg}$ are placed. The mass of the elements of the autoclave internal structure is $m_{\text{zvk}}=22 \times 10^3 \text{ kg}$.

The following are accepted as the initial conditions:
1) The temperatures of the raw concretes placed in the autoclave and the elements of the internal structure of the autoclave are uniform across the volume and $T_0$ equals to $70^\circ\text{C}$;
2) Air has been completely forced out of the pores of cellular concrete and the internal environment of the autoclave;
3) The initial steam pressure in the autoclave $P_0=56 \times 10^3 \text{ Pa}$. 
Assumptions:
1. We consider that each raw concrete is a plate uniformly treated with steam along all the surfaces. Taking into account that \(2R\) plate thickness is 0.64 m, where \(R=0.32\) m, we assume it a thin body in terms of heating;
2. We assume that, given the large inertia of the process, the temperature of the raw concrete \(T_m\) is equal to the temperature of the internal environment of the autoclave \(T_{aut}\);
3. We believe that the transfer of heat to the raw concretes, determined by the supply of saturated steam to the autoclave, is carried out by means of convective heat exchange and steam condensation on the surfaces of products and elements of the internal structure of the autoclave. Moreover, we take into account that, starting from a temperature \(T\) value of \(165^\circ C\), internal heat generation occurs in autoclaved products due to the chemical reaction of the formation of calcium hydroxides in the structure of the raw concrete;
4. We assume that the process of internal heat generation is determined by the formation of hydroxides only in the form of tobermorite, and its dynamics can be represented by a symmetric smooth curve [4];
5. We believe that we are aware of the range of values of the main characteristics describing the chemical and mineralogical composition of steamed raw cellular concretes of a given density grade;

3. Mathematical Description
As applied to the task, within the accepted assumptions, the heat exchange processes in the autoclave can be represented, in the first approximation, as an object with lumped parameters. In this case, the raw cellular concretes are presented in the form of thermally thin bodies (plates). The plate is heated by the total heat flow, for which the heat balance equation holds true:

\[
F = F_m + F_{tb} - F_{ok} - F_0, \tag{1}
\]

where \(F_m, F_{tb}, F_{ok}, F_0\) are the heat flows generated in the autoclave by \(g_n\) flow rate of steam from the main line, heat generation in the raw cellular concretes during the formation of hydroxides, losses through the protective covering and steam consumption for filling the autoclave to a given pressure, respectively.

Heat transfer from steam to the raw concretes during their autoclave treatment is carried out both by means of convective heat exchange [5] and by heat transfer [6]. The resulting heat flow is represented by their sum:

\[
F_m = F_n + F_k, \tag{2}
\]

where \(F_n\) is the thermal capacity released during steam condensation, \(F_k\) is the residual heat of hot condensate. Convective heat transfer, which characterizes the transfer of heat from steam to the concretes during condensation, is described by the equation:

\[
F_n = g_n r_n, \tag{3}
\]

where \(g_n\) is the steam consumption, \(r_n\) is the specific heat of vaporization. Heat transfer from condensate to raw cellular concretes can be described as (Fourier thermal conductivity law):

\[
F_k = a(T_k - T_m)S, \tag{4}
\]

where \(a\) is the heat transfer coefficient, \(T_k\) and \(T_m\) are the vapor condensation temperature (a non-stationary characteristic described by \(f(P_{abs})\) function of the pressure in the autoclave) and the temperature of the raw cellular concrete, respectively, \(S\) is the surface area involved in heat exchange for 12 considered raw concrete blocks with \(S=300\) m².

Steam is supplied to the autoclave through an adjustable main valve, and is discharged by means of a steam battery valve and a relief valve together making up the system of controlled valves. Thus, steam flow rate, which determines the value \(F_n\) is presented by:

\[
g_n = g_{m} - g_{ok} - g_{ab}, \tag{5}
\]
where the flow through the corresponding valve is determined by the ratio of pressure in a given area to its hydraulic resistance \( g_m = P_m/R_{gm} \), \( g_{akk} = P_{akk}/R_{gakk} \), and \( g_{nk} \) flow rate is constant when the condition \( P_{abt} \geq P_{max} \) is met.

The heat flow of internal heat generation in raw cellular concretes during the formation of tobermorite \( F_{tb} \) seems to be a symmetrical smooth curve, with the accepted assumptions:

\[
F_{tb} = Q_{tb}/(2t_1 + t_2),
\]

(5)

here \( Q \) is the amount of heat, \( t_1 \) and \( t_2 \) are the time intervals characterizing the intensity of heat release.

\( F_{ok} \) value of heat loss through protective covering in accordance with Fourier law of heat conduction is:

\[
F_{ok} = \lambda S(T_{abt} - T_{nap})/l,
\]

(6)

where \( \lambda \), \( S \), \( l \) are the coefficient of thermal conductivity, surface area and wall (lining) thickness of the autoclave, \( T_{abt} \), \( T_{nap} \) are the temperatures inside the autoclave and the environment, respectively.

The amount of heat needed to create pressure in the autoclave:

\[
F_0 = g_0 r_n,
\]

(7)

where \( g_0 \) is steam consumption at the stage of pressure rise.

Thermal power \( \Phi \) is used for heating raw cellular concrete \( F_b \) and steel elements of the internal structure of the autoclave \( F_{ct} \):

\[
\Phi = F_b + F_{ct},
\]

(8)

Where \( F_b = c_b m_b \frac{dT_{abt}}{dt} \) and \( F_{ct} = c_{ct} m_{ct} \frac{dT_{abt}}{dt} \), here the values of \( c_b \), \( c_{ct} \), \( m_b \), \( m_{ct} \) are the heat capacity, the mass of autoclaved concrete and steel elements of the internal structure of the autoclave, respectively.

Taking into account the accepted assumptions, the heat balance equation can be written in the form of the well-known Fourier-Kirchhoff convective heat exchange equation:

\[
c_b m_b \frac{dT_{abt}}{dt} + c_{ct} m_{ct} \frac{dT_{abt}}{dt} = g_n r_n + \alpha S(T_k - T_m) + \frac{Q_{tb}}{2(t_1 - t_2)} - \frac{\lambda S(T_{abt} - T_{nap})}{l} - g_0 r_n,
\]

(9)

However, the process of autoclaving is controlled by using a regulator for a given programmed trajectory of \( P_{abt} \) pressure in the autoclave, whereas an observer of temperature \( P_{abt} \) is needed only to comply with the restrictions imposed on the pressure increase stage. In relation to the task, \( P_{abt} \) pressure in the autoclave can be obtained from the equation of state of an ideal gas.

Based on the obtained equations, the structure of the mathematical model of the autoclave treatment process as an object with lumped parameters was synthesized (Figure 1).
Figure 1. The structure of the mathematical model of the process of autoclave treatment as a control object.

Based on the proposed mathematical model, a computational model was developed using Matlab software (Figure 2).

Figure 2. Computational model of the control object with lumped parameters.

The input of the system has $g_n=0.1 \text{ kg/s}$ flow rate of the steam line with stepped effect for $t_1=11700 \text{ s}$, which corresponds to the duration of the pressure rise in the autoclave. Let us perform a series of experimental investigations of the control object with and without heat losses through the protective covers of the autoclave $F_{ok}$ and the heat flow from the internal heat release $F_{ib}$ as applied to D400 grade concrete. As a result, at the output of the control object, we obtain a family of pressure curves $P_{abt}$ (Figure 3) and temperature in an autoclave $T_{abt}$ (Figure 4) under given conditions.
Figure 3. $P_{abt}$ pressure curves in the autoclave: 1 – without loss of $F_{ok}$ or $F_{tb}$ heat release; 2 – with losses of $F_{ok}$ without $F_{tb}$ heat release; 3 – with losses of $F_{ok}$ and $F_{tb}$ heat release.

Similarly, $T_{abt}$ temperature curves in an autoclave for D500 and D600 grade concrete are formed (Figure 5).

Figure 4. $P_{abt}$ pressure curves in the autoclave. 1 – without loss of $F_{ok}$ or $F_{tb}$ heat release; 2 – with losses of $F_{ok}$ without $F_{tb}$ heat release; 3 – with losses of $F_{ok}$ and $F_{tb}$ heat release.

The curves obtained in the computational model quite accurately coincide with the production data given in [3], which confirms the adequacy of the developed model.
Figure 5. \( \text{T}_{\text{abt}} \) curves for temperature in an autoclave for autoclaved concretes by density grade: 1 – D400; 2 – D500; 3 – D600.

At the second stage of modeling, to find the temperature field \( T_{m}(x,y,z,t) \) of the raw cellular concrete, at the stage of pressure increase and curing in the autoclave, we consider the D400 concrete, with measurements of 6x1.3x0.64 m. The concrete is placed into the saturated steam environment, the temperature \( T_{n} \) of which varies as a function of time and is assumed to be equal to the temperature \( T_{\text{abt}} \) without taking into account the internal heat generation (Figure 4, 2) determined at the first stage of modeling. The temperature dynamics \( T_{n}(t) \), the initial pressure \( P_{n}^{0} \) of steam environment and the initial temperature distribution \( T_{m}^{0}(x,y,z,0) \) over the volume of the concrete are set as initial conditions, with the initial pressure \( P_{n}^{0} = 0.056 \text{ MPa} \), and the initial temperature distribution over the volume of the concrete being uniform and having the value \( T_{m}^{0}(x,y,z,0) = 70^\circ \text{C} \). The heat capacity and density of the raw concrete are determined by analogy with [7]. The thermal conductivity of raw concretes \( \lambda_{m} \) in the process of their autoclave treatment, obviously, differs from the grade value. Well-known experimental studies [8] present the data on the influence of well-defined factors on the heat transfer process in cellular concretes. The authors of the above-mentioned studies found that heating of autoclaved products largely depends on mass transfer, the intensity of which, in turn, depends on the presence of air in the pores of raw concretes, which impedes heat and mass transfer processes. The relationship of mass transfer coefficients and thermal conductivity can be determined by the expression [9]:

\[
\beta = \frac{\alpha}{c_{p} \rho_{m}}, \tag{10}
\]

where \( c_{p} \) is the specific heat capacity of the concretes, \( \rho_{m} \) is the density of the concretes, \( \alpha \) is the heat transfer coefficient, equal to the ratio of the concretes thermal conductivity \( \lambda_{m} \) to the thickness of the boundary layer \( \delta \):

\[
\alpha = \frac{\lambda_{m}}{\delta}, \tag{11}
\]

The value \( \beta \) of the mass transfer coefficient for the autoclave processing of cellular concrete can be determined by jointly solving the differential equations of mass transfer [10], Navier-Stokes and continuity equations, or by conducting field experiments. Applied to this problem, an approximate value of \( \beta \) can be taken by analogy with [8]. Then, within the framework of the accepted assumptions, we suppose that \( \lambda_{m} \) value of thermal conductivity of concretes takes the value equivalent to \( \lambda_{m}^{\varepsilon} \), taking into account the mass exchange between steam and raw cellular concrete.

Internal heat generation is defined as a volume heat source, the dynamics of the specific volume heat generation of which is determined in accordance with [4], and its value:
\[ q_{\text{tb}} = \frac{Q_{\text{max}}}{12}, \quad (12) \]

where \( Q_{\text{max}} \) is the maximum heat generation value for 12 concretes. It is known [3] that the internal heat generation in cellular concrete during its autoclave treatment is due to the exothermic reaction of tobermorite formation in its structure. The reaction starts when the raw cellular concrete reaches \( T_{\text{t}} \) temperature. Let us set the value of 165ºC for \( T_{\text{t}} \) as a target set point, reaching which a volume heat source with the specified magnitude and volume specific heat dynamics previously described is generated within the raw concrete.

Let us conduct a number of computational experiments using SolidWorks *Flow simulation* software. The physical calculation time corresponds to the duration of the stages of pressure increase and curing, summing up to \( t_p = 36000 \) s.

![Figure 6. Dynamics of \( T_m(x, y, z, t) \) temperature: 1 – on the surface of raw concrete; 2 – at \( \frac{1}{4} \) thickness of the raw concrete; 3 – in the center of concrete](image)

As a result of computational experiments, the temperature dynamics \( T_m(x, y, z, t) \) in the most characteristic parts of the cellular concrete was determined on the model (Figure 6). The results of modeling thermal processes in raw cellular concrete with a sufficient degree of accuracy coincide with the data given in [3, 8], which proves the adequacy of the developed mathematical model.

4. Conclusion
The mathematical and computational model of the autoclave processing as a control object in the assumption of the concentration of parameters has been developed. The temperature dynamics of steam in an autoclave \( T_n(t) \) has been determined. Computational experiments were carried out to determine \( T_m(x, y, z, t) \) temperature dynamics at the most characteristic parts of the cellular concrete as an object with distributed parameters, taking into account the internal heat release during the formation of tobermorite. The assessment of the adequacy of the developed model was made by comparing the results of modeling with the results of experimental studies obtained with the existing process equipment.
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