Mathematical modelling and development of a computational algorithm for the study of thermo-stressed state of a heat-resistant alloy

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ABSTRACT

The problem of increasing the thermal stability of structural elements made of heat-resistant metals and alloys operating in a complex force and thermal field is one of the key priorities of modern high technology research. The most important case is the study of the thermal stability of structural elements in real conditions of heat fluxes with varying intensity, with a complex configuration of heat-insulated local surfaces and internal point heat sources. Many basic load-bearing structural elements operating in a large thermal field (elements of gas turbine and jet engines, etc.), are made of heat-resistant alloys. The physical feature of such alloys is that the coefficient of thermal expansion and the modulus of elasticity of the material strictly depends on the temperature distribution field, that is, the coefficients are a function of temperature. The purpose of this study is to simulate a thermo-stressed state in rod elements of a structure based on the law of conservation of energy, in the presence of a heat flux applied on the lateral surface, which varies along the coordinate in a linear manner. To solve the outlined problem, a potential energy minimisation method is used in combination of a quadratic finite element with three nodes. As a result, from the condition of the minimum of the functional defining the potential energy, a resolving system of linear algebraic equations is obtained. All possible natural boundary conditions are taken into account. In this system, all integrals used are calculated analytically. Moreover, the law of conservation of energy is fulfilled for each of the equations of the resulting system. As a result, the values of displacement, deformation and stresses were calculated, as well as the values of elastic temperature and thermoelastic components of deformations and stresses for a specific example.

Keywords: Thermal expansion, Modulus of elasticity, Thermal stress state, Displacement discretisation, Stress strain.

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1. Introduction

Modern internal combustion engines, gas turbine power plants, oil heating compressor stations, steam generators of nuclear reactors, and technological processes that allow the deep processing of uranium and osmium ores, as well as crude oil, pose the urgent problem of developing a mathematical model for studying the temperature distribution field of thermal, physico-mechanical state of the bearing elements of these structures, taking into account the nonlinear physical properties of materials and their operating conditions. In all technological processes, the load-bearing elements of these structures are made of heat-resistant alloys. Therefore, in the field of metallurgical science, favourable conditions are created for the production of more advanced heat-resistant alloys with high resistance to plastic deformation and fracture under the influence of



high temperatures [1-15].

It is known that in a thermo-physical-mechanical process, the main characteristic that has a significant effect on the strength of load-bearing structural elements is an intense temperature rise, i.e., heat flux. In general, temperature is one of the most important characteristics of the growth process and affects the morphology and crystal structure of heat-resistant alloys. In different parts of the alloy, the distribution of the temperature field is uneven [16]. Consequently, during the thermomechanical process, in some areas of the structural elements, the temperature will be acceptable, and in some areas – critical, which leads to rapid wear of the structural elements and to the loss of their physical qualities. In this regard, for an accurate calculation of the distribution of the temperature field over the volume of multidimensional bodies of various configurations made of heatresistant alloys, it is necessary to carry out effective theoretical and numerical modelling [17-30].

The purpose of modelling, both analytical and imitation, is to predict the state of the system, which most realistically displays the picture of the temperature field distribution over the volume of a multidimensional body. [31]. In the long term, based on this forecast, by changing both the internal parameters of the structure of structural elements and the characteristics of external influences, it will be possible to determine all the vulnerabilities in the structural elements and protect them from deformation or destruction. The development of a model of the temperature distribution over the body volume is necessary, since the complexity of the thermomechanical process in real time greatly reduces the ability to intuitively assess the identification of critical temperatures in body parts. Therefore, theoretical modelling of the temperature distribution over the volume of multidimensional bodies of various configurations made of heat-resistant alloys is undoubtedly an urgent problem.

2. Material and methods

In the case of a nonlinear one-dimensional and two-dimensional problem, the numerical simulation of the temperature distribution field in a fixed cross section is determined when the investigated temperature process depends on the applied heat flux, material length, the heat transfer coefficient, and the ambient temperature. Using all this data by the method of minimising potential energy in combination of a quadratic finite element with three nodes, the thermo-stressed state of the material is numerically assessed in the presence of a heat flux on the lateral surface, which varies along the coordinate in a linear manner.

To calculate the temperature stresses in structural elements, it is necessary to determine the temperature distribution law in the investigated elements. As known, the equation of heat conduction in a continuous medium has the form [32-45] (Eq. 1):

$$K_{xx}\frac{\partial^2 T}{\partial x^2} + K_{yy}\frac{\partial^2 T}{\partial y^2} + K_{zz}\frac{\partial^2 T}{\partial z^2} + Q = 0,$$
(1)

where T(x, y, z) – temperature, the dimension of which is $\cdot C$; K_{xxx}, K_{yy}, K_{zz} – coefficient of thermal conductivity (of the body material) in directions x, y, z, dimensions $W/(cm \cdot C)$; Q – a heat source inside the body, which is considered positive if heat is applied to the body W/cm^3 . or equation (1), the following boundary conditions hold: if the temperature is known at the points of the surface S_1 then on this surface the boundary conditions will be (Eq. 2):

$$T = T_s(S_1) \rightleftharpoons \text{ for } S_1, \tag{2}$$

where T_{s} - set temperature at the boundary, which can be a function of the coordinates of the surface point S_1 . If convective heat transfer passes through the surface S_2 , which is characterised by the value $h(T - T_{OC})$, then for points of this surface the boundary conditions have the form (Eq. 3):

$$K_{xx}\frac{\partial T}{\partial x}l_x + K_{yy}\frac{\partial T}{\partial y}l_y + K_{zz}\frac{\partial T}{\partial z}l_z + h(T - T_{oc}) = 0 \text{ for } S_2$$
(3)

where h – heat transfer coefficient, $(W/(cm^2 \cdot C))$ and this coefficient can be a function of the coordinates of the points of the surface S_2 ; T(x, y, z) – temperature at points of the surface S_2 , the value of which is unknown; T_a – set temperature of the surrounding surface S_2 of the environment. It can also be a function of

the coordinates of points on the surface S_2 ; l_x, l_y, l_z - direction cosines of surface S_2 . If the heat flux q, $W/(cm \cdot C)$ is applied to the surface S_2 of the body, then (Eq. 4) holds for points of this surface:

$$K_{xx}\frac{\partial T}{\partial x}\ell_x + K_{yy}\frac{\partial T}{\partial y}\ell_y + K_{zz}\frac{\partial T}{\partial z}\ell_z + q = 0 \text{ for } S_3.$$
(4)

The given heat flux q can be a function of the coordinates of the points of the surface S_3 . It should be noted here that the heat flux q and convective heat loss $h(T - T_{oc})$ do not occur on the same area of the boundary surface. This means that if there is heat loss due to convection, then there is a removal or inflow of heat due to the heat flux and vice versa. Thus, equation (1) with the reduced boundary conditions (2)-(3) has a unique solution. This solution is the law of temperature distribution in the body. But in the calculus of variations [46; 47; 48-56], it is established that solving equation (1) with boundary conditions (2)-(4) is equivalent to finding the minimum of the functional (Eq. 5):

$$J = \int_{V_{2}} \frac{1}{2} \left[K_{xx} \left(\frac{\partial T}{\partial x} \right)^{2} + K_{yy} \left(\frac{\partial T}{\partial y} \right)^{2} + K_{zz} \left(\frac{\partial T}{\partial z} \right)^{2} - 2Q \cdot T \right] dV + \int_{S_{2}} \frac{h}{2} (T - T_{oc})^{2} dS + \int_{S_{8}} qT dS.$$
(5)

In addition, equation (1) and boundary conditions (2)-(4) can be applied to one-dimensional problems by simply deleting the terms associated with unnecessary coordinates. Then the equation for the one-dimensional problem is written in the form (Eq. 6):

$$K_{xx}\frac{\partial^2 T}{\partial x^2} + Q = 0, \tag{6}$$

with the corresponding boundary conditions (Eq. 7-9):

$$T = T_3 \text{ for } S_1, \tag{7}$$

$$K_{xx}\frac{\partial T}{\partial x}\ell_x + h(T - T_{OC}) = 0 \text{ for } S_2,$$
(8)

$$K_{xx}\frac{\partial T}{\partial x}\ell_x + q = 0 \quad \text{for } S_3. \tag{9}$$

If there is no convective heat transfer and, in addition, the heat flux is zero, then equations (8), (9) are reduced to (Eq. 10):

$$\frac{dT}{dn} = 0, \tag{10}$$

which expresses the condition for the existence of a thermally insulated boundary. Here n – outward normal. In the calculus of variations, it is established that to minimise the functional (Eq. 11):

$$J = \int_{V} \frac{K_{xx}}{2} \left(\frac{\partial T}{\partial x}\right)^{2} dV + \int_{S_{2}} \frac{h}{2} (T - T_{oc})^{2} dS + \int_{S_{g}} qT dS,$$
(11)

it is necessary that the differential equation (6) and boundary conditions (7)-(9) are satisfied. Therefore, any temperature distribution field at which functional (11) becomes minimal also satisfies differential equations and thus is a solution to the posed problem.

3. Results and discussion

Using this statement, the thermo-stressed state of the material of the body (rod) is investigated. This study is devoted to mathematical modelling and the development of an appropriate computational algorithm for studying the thermo-stressed state of a rod clamped by two ends. On the lateral surface of the rod, a heat flux is applied, varying along the coordinate linearly [57; 58-66] (Eq. 12):

$$q(x) = ax + b, \tag{12}$$

a, b = const – real numbers. In order to numerically study the thermo-physical-mechanical phenomena of the alloy material, take a rod of length l(cm), the cross-sectional area $F[cm^2]$ – is constant along the length of rod. The physical and mechanical properties of the rod material are characterised by the modulus of elasticity $E\left[\frac{kg}{cm^2}\right]$, the coefficient of thermal expansion $\alpha\left(\frac{1}{cc}\right)$, heat exchange with the environment $h\left[\frac{W}{cm^2\cdot C}\right]$ and thermal conductivity $K_{xex}\left(\frac{W}{cm^2\cdot C}\right)$. Through the cross-sectional areas of the two clamped ends, heat exchange of different intensities occurs with the media surrounding them. The heat transfer coefficient for the left end of the rod is denoted by $h_0\left[\frac{W}{(cm^2\cdot C)}\right]$, and the temperature of the environment surrounding this area – $T_{oc}(^{\circ}C)$, and for the right end, respectively – $h_1\left[\frac{W}{(cm^2\cdot C)}\right]$ and $T_{ocl}(^{\circ}C)$. The diagram scheme for this problem is presented in Figure 1.



Figure 1. Analytical model

The rod heats up due to the action on the lateral surface of a given heat flux $q(x)(\frac{W}{cm^2})$. In this regard, it is expanding. Since both ends of the rod are rigidly restrained, it cannot be lengthened. In this regard, a compressive force R(kg(f)), arises at the two ends of the rod, which leads to the appearance of a stress σ , $(kg(f)/cm^2)$ in the sections of the rod. Such a task is called statically indeterminate. Despite this, this problem can be solved numerically if the potential energy minimisation method is used in combination with a quadratic finite element with three nodes. The equation of potential energy for the considered problem is defined as follows [67; 68; 69-80] (Eq. 13):

$$\Pi = \int_{V} \frac{\sigma_{x} \cdot \varepsilon_{x}}{2} dv - \int_{V} \alpha \cdot E \cdot T(X) \cdot \varepsilon_{x} dv, \qquad (13)$$

where V, (cm^3) – volume of the considered bearing rod element; u(x), (cm) – displacement distribution field of the cross section of the rod; field distribution of elastic component of deformation (longitudinal deformation) (Eq. 14)

$$\varepsilon_x = \frac{\partial u}{\partial x};$$
 (14)

the field of distribution of the elastic component of the compression-tension stress (Eq. 15-16);

$$\sigma_x = E, \tag{15}$$

$$\varepsilon_x = E \cdot \frac{\partial u}{\partial x} (kg(f)/cm^2); \tag{16}$$

field distribution of the elasticity modulus of the material of the rod element (17):

$$E=E(T(x)) \tag{17}$$

and $\alpha(T(x))$ – field of distribution of the coefficient of thermal expansion of the material of the rod element, which depend on temperature; temperature distribution law along the length of the bearing element (Eq. 18):

$$T = T(x), \tag{18}$$

which is approximated by a complete second-order polynomial, i.e., [81; 82; 83; 84-102] (Eq. 19):

$$T(x) = ax^{2} + bx + c; \text{ at } 0 \le x \le l,$$
(19)

where a, b, c – some constants whose values are still unknown. To find the value of these constants, divide the considered part of the rod in half. And in this part three nodes (i, j, k) are fixed (Figure 2).



Figure 2. One-dimensional quadratic finite element

The global coordinates of these nodes are respectively x_i, x_j, x_k , while (Eq. 20):

$$x_j = \frac{x_l + x_k}{2}.\tag{20}$$

In this case, in the local system, the coordinates of the three nodes are determined as follows (Eq. 21-23):

$$\boldsymbol{x}_i = \boldsymbol{0}; \tag{21}$$

$$x_j = \frac{\ell}{2}; \tag{22}$$

$$x_k = \ell. \tag{23}$$

Next, introduce the following notation characterising the temperature value at nodes i, j, k (Eq. 24):

$$T_i = T(x = x_i); \quad T_j = T(x = x_j); \quad T_k = T(x = x_k).$$
 (24)

Then, substituting (24) into (19), a system of three equations is composed to determine the values of the constants a, b, c (Eq. 25):

$$\begin{array}{l} ax_{i}^{2} + bx_{i} + c = T_{i}; \\ ax_{j}^{2} + bx_{j} + c = T_{j}; \\ ax_{k}^{2} + bx_{k} + c = T_{k}; \end{array} \right\}$$
(25)

taking into account that (21)-(23), from the last system obtain (Eq. 26):

$$c = T_{i};
\frac{\ell^{2}}{4}a + \frac{\ell}{2}b + c = T_{j};
\ell^{2}a + \ell b + c = T_{k}.$$
(26)

Considering that (Eq. 27):

$$\boldsymbol{c} = \boldsymbol{T}_i,\tag{27}$$

from the last two equations of system (26) obtain (28):

$$\frac{\ell^2}{4}a + \frac{\ell}{2}b = T_j - T_i; \\ \ell^2 a + \ell b = T_k - T_i. \end{cases}$$
(28)

From here it follows (Eq. 29):

$$a = \frac{2(T_k - 2T_j + T_i)}{\ell^2};$$

$$b = \frac{4T_j - T_k - 3T_i}{\ell};$$

$$c = T_i.$$
(29)

Substituting the obtained values of *a*, *b*, *c* into (19), obtain (Eq. 30):

$$T(x) = \frac{(2T_k - 4T_j + 2T_i)}{\ell^2} x^2 + \frac{(4T_j - T_k - 3T_i)}{\ell} x + T_i = \frac{\ell^2 - 3\ell x + 2x^2}{\ell^2} T_i + \frac{4\ell x - 4x^2}{\ell^2} T_j + \frac{2x^2 - \ell x}{\ell^2} T_k$$
(30)

Let us introduce the following equation (31):

$$\begin{array}{l}
\phi_{i}(x) = \frac{\ell^{2} - 3\ell x + 2x^{2}}{\ell^{2}}; \\
\phi_{j}(x) = \frac{4\ell x - 4x^{2}}{\ell^{2}}; \\
\phi_{k}(x) = \frac{2x^{2} - \ell x}{\ell^{2}}.
\end{array}$$
(31)

Then, taking into account (31), rewrite (30) in the following form (32):

$$T(x) = \phi_i(x)T_i + \phi_j(x)T_j + \phi_k(x)T_k, \text{ at } 0 \le x \le \ell,$$
(32)

where the functions $\phi_i(x)$, $\phi_j(x)$, $\phi_k(x)$ are called form functions for a one-dimensional quadratic finite element with three nodes. It should be noted that these form functions have certain properties. Now consider the properties of these form functions (Eq. 33-34):

$$\begin{array}{l} \phi_i(x)|_{x=x_i} = \phi_i(x=x_i=0) = 1; \\ \phi_j(x)|_{x=x_i} = \phi_j(x=x_i=0) = 0; \\ \phi_k(x)|_{x=x_i} = \phi_k(x=x_i=0) = 0. \end{array} \right\},$$
(33)

$$\begin{aligned} \phi_i(x)|_{x=x_j} &= \phi_i(x=x_j=\frac{\ell}{2}) = 0; \\ \phi_j(x)|_{x=x_j} &= \phi_j(x=x_j=\frac{\ell}{2}) = 1; \\ \phi_k(x)|_{x=x_j} &= \phi_k(x=x_j=\frac{\ell}{2}) = 0. \end{aligned}$$
(34)

$$\begin{aligned} \phi_i(x)|_{x=x_k} &= \phi_i(x=\ell) = 0; \\ \phi_j(x)|_{x=x_k} &= \phi_j(x=\ell) = 0; \\ \phi_k(x)|_{x=x_k} &= \phi_k(x=\ell) = 1. \end{aligned}$$
(35)

In addition, for any point of (Eq. 36):

$$x = x_{\phi} \tag{36}$$

in the range $0 \le x \le \ell$ one has (Eq. 37):

$$\phi_i(x_{\phi}) + \phi_j(x_{\phi}) + \phi_k(x_{\phi}) = 1.$$
(37)

For example (Eq. 38):

$$x_{\phi} = \frac{\ell}{4}.$$
(38)

Then (Eq. 39):

$$\phi_i(x_{\phi}) + \phi_j(x_{\phi}) + \phi_k(x_{\phi}) = \frac{\ell^2 - 3\ell_{\frac{1}{4}+2}^{\ell} \frac{\ell^2}{16}}{\ell^2} + \frac{4\ell_{\frac{1}{4}-4}^{\ell} \frac{\ell^2}{16}}{\ell^2} + \frac{2\ell_{\frac{1}{4}-2}^{\ell} \ell_{\frac{1}{4}}}{\ell^2} = \frac{3}{8} + \frac{3}{4} - \frac{1}{8} = \frac{3+6-1}{8} = 1$$
(39)

Also, form functions have the following properties. For any point of the interval $0 \le x \le l$, i.e., within each finite element one has (Eq. 40):

$$\frac{\partial \phi_i(x)}{\partial x} + \frac{\partial \phi_j(x)}{\partial x} + \frac{\partial \phi_k(x)}{\partial x} = 0.$$
(40)

Using equation (31), prove (Eq. 41):

$$\frac{\partial \phi_i(x)}{\partial x} = \frac{1}{\ell^2} (-3\ell + 4x);$$

$$\frac{\partial \phi_j(x)}{\partial x} = \frac{4}{\ell^2} (\ell - 2x);$$

$$\frac{\partial \phi_k(x)}{\partial x} = \frac{1}{\ell^2} (4x - \ell).$$
(41)

Next, find the total (Eq. 42):

$$\frac{\partial \phi_i(x)}{\partial x} + \frac{\partial \phi_j(x)}{\partial x} + \frac{\partial \phi_k(x)}{\partial x} = \frac{1}{\ell^2} \left[-3\ell + 4x + 4\ell - 8x + 4x - \ell \right] = 0.$$
(42)

Within the length of the element under consideration, the displacement distribution field (Eq. 43):

$$u = u(x), \tag{43}$$

approximating by a second-order polynomial, obtain (Eq. 44):

$$u = u(x) = \varphi_i(x) \cdot u_i + \varphi_j(u_j) + \varphi_k(x) \cdot u_k, \tag{44}$$

where u_i , u_j , u_k – displacements of the section of the rod, the coordinates of which (Eq. 45):

$$x = 0; \ x = \frac{l}{2}; x = l.$$
 (45)

Then, within the limits of the length of the rod (the element under consideration), the displacement gradient, i.e., the distribution field of the elastic component of deformation (ε_x) is expressed as follows (Eq. 46):

$$\varepsilon_x = \frac{\partial u}{\partial x} = \frac{\partial \varphi_i(x)}{\partial x} u_i + \frac{\partial \varphi_j(x)}{\partial x} u_j + \frac{\partial \varphi_k(x)}{\partial x} u_k.$$
(46)

Based on Hooke's law, the value of the elastic stress component is determined as follows (Eq. 47):

$$\sigma_x = E \cdot \varepsilon_x = E \cdot \left(\frac{4x - 3l}{l^2} u_i + \frac{4l - 8x}{l^2} u_j + \frac{4x - l}{l^2} u_k\right) \tag{47}$$

According to the theory of thermoelasticity, the values of deformation from the temperature field are determined by the equation (Eq. 48):

$$\varepsilon_T = -\alpha T(x). \tag{48}$$

The values of the temperature component of the voltage are determined by the equation (Eq. 49):

$$\sigma_T = \mathbf{E} \cdot \boldsymbol{\varepsilon}_T \,, \tag{49}$$

a of thermoelastic stress (Eq. 50):

$$\sigma = \sigma_x + \sigma_T. \tag{50}$$

The cross-sectional area of the rod $F(cm^2)$ is constant along the length, equation (13) is written in the following form (Eq. 51):

$$\Pi = \int_{V} \frac{\sigma_{x}}{2} \cdot \varepsilon_{x} \cdot dv - \int_{V} \alpha \cdot E \cdot T(x) \cdot \varepsilon_{x} \cdot dv =$$

$$= \frac{F}{2} \int_{0}^{l} \sigma_{x} \cdot \varepsilon_{x} dx - F \cdot \int_{o}^{l} \alpha \cdot E \cdot T(x) \cdot \varepsilon_{x} \cdot dx =$$

$$= \frac{E \cdot F}{2} \int_{0}^{l} \varepsilon_{x}^{2} \cdot dx - \alpha \cdot E \cdot F \cdot \int_{0}^{l} T(x) \cdot \varepsilon_{x} \cdot dx; \qquad (51)$$

In order to improve the accuracy and improve the convergence of the obtained numerical results, two intergrades are analytically integrated in volume (52):

$$\begin{split} \Pi &= \frac{E}{2} \int_{V} \varepsilon_{x}^{2} dV - \alpha E \int_{V} T(x) \varepsilon_{x} dV = \frac{EF}{2} \int_{0}^{\ell} \varepsilon_{x}^{2} dx - \alpha EF \int_{0}^{\ell} T(x) \varepsilon_{x} dx = \\ &= \frac{EF}{2\ell^{4}} \left\{ \left[\frac{16x^{3}}{3} - 12\ell x^{2} + 9\ell^{2} x \right] u_{i}^{2} + 2 \left[20\ell x^{2} - \frac{32x^{3}}{3} - 12\ell^{2} x \right] u_{i} u_{j} + 2 \left[\frac{16x^{3}}{3} - 8\ell x^{2} + 3\ell^{2} x \right] u_{i} u_{k} + \\ &+ \left[16\ell^{2} x - 32\ell x^{2} - \frac{64x^{3}}{3} \right] u_{j}^{2} + 2 \left[12\ell x^{2} - \frac{32x^{3}}{3} - 4\ell^{2} x \right] u_{j} u_{k} + \left[\frac{16x^{3}}{3} - 4\ell x^{2} + \ell^{2} x \right] u_{k}^{2} \right] \right\}_{0}^{\ell} - \\ &- \frac{\alpha EF}{\ell^{4}} \left\{ \left[\frac{13\ell^{2}x^{2}}{2} - 6\ell x^{3} - 3\ell^{3} x + 2x^{4} \right] T_{i} u_{i} + \left[\frac{32\ell x^{3}}{3} - 10\ell^{2} x^{2} + 4\ell^{3} x - 4x^{4} \right] T_{i} u_{j} + \\ &+ \left[\frac{7\ell^{2}x^{2}}{2} - \frac{14\ell x^{3}}{3} - \ell^{3} x + 2x^{4} \right] T_{i} u_{k} + \left[\frac{28\ell x^{3}}{3} - 6\ell^{2} x^{2} + 4x^{4} \right] T_{j} u_{i} + \left[8\ell^{2} x^{2} - 16\ell x^{3} + 8x^{4} \right] T_{j} u_{j} + \\ &+ \left[\frac{20\ell x^{3}}{3} - 2\ell^{2} x^{2} - 4x^{4} \right] T_{j} u_{k} + \left[\frac{32\ell^{2} x^{2}}{2} - \frac{10\ell x^{3}}{3} + 2x^{4} \right] T_{k} u_{i} + \left[\frac{16\ell x^{3}}{3} - 2\ell^{2} x^{2} - 4x^{4} \right] T_{k} u_{j} + \\ &+ \left[\frac{\ell^{2} x^{2}}{2} - 2\ell x^{3} + 2x^{4} \right] T_{k} u_{k} \right]_{0}^{\ell} = \frac{EF}{6\ell} \left[7u_{i}^{2} - 16u_{i} u_{j} + 2u_{i} u_{k} + 16u_{j}^{2} - 16u_{j} u_{k} + 7u_{k}^{2} \right] - \\ &- \frac{\alpha EF}{6} \left[-3T_{i} u_{i} + 4T_{i} u_{j} - T_{i} u_{k} - 4T_{j} u_{i} + 4T_{i} u_{j} - 4T_{k} u_{j} + 3T_{k} u_{k} \right]$$

$$(52)$$

It should be noted here that the total of the coefficients in square brackets is zero. This shows the convergence of the obtained numerical results. Using the obtained calculations in equation (52), it is possible to write the final integrated form of the potential energy formula (Eq. 53):

$$\Pi = \frac{EF}{6l} \left[7u_i^2 - 16u_i u_j + 2u_i u_k + 16u_j^2 - 16u_j u_k + 7u_k^2 \right] - \frac{\alpha \cdot E \cdot F}{6} \left[-3T_i u_i + 4T_i u_j - T_i u_k - 4T_j u_i + 4T_j u_k + T_k u_i - 4T_k u_j + +3T_k u_k \right]$$
(53)

Considering that the nodal temperature values are known, the potential energy will be minimised by the nodal displacement values. As a result, obtain a system of linear algebraic equations (Eq. 54):

$$1) \frac{\partial \Pi}{\partial u_{i}} = 0 \Longrightarrow \frac{7EF}{3l} u_{i} - \frac{8EF}{3l} u_{j} + \frac{EF}{3l} u_{k} = -\frac{\alpha EF}{2} T_{i} - \frac{2\alpha EF}{3} T_{j} + \frac{\alpha EF}{6} T_{k};$$

$$2) \frac{\partial \Pi}{\partial u_{j}} = 0 \Longrightarrow -\frac{8EF}{3l} u_{i} + \frac{16EF}{3l} u_{j} - \frac{8EF}{3l} u_{k} = \frac{2\alpha EF}{3} T_{i} - \frac{2\alpha EF}{3} T_{k};$$

$$3) \frac{\partial \Pi}{\partial u_{k}} = 0 \Longrightarrow \frac{EF}{3l} u_{i} - \frac{8EF}{3l} u_{j} + \frac{7EF}{3l} u_{k} = -\frac{\alpha EF}{6} T_{i} + \frac{2\alpha EF}{3} T_{j} + \frac{\alpha EF}{2} T_{k}.$$

$$(54)$$

To test the developed computational algorithm, the following test problem is taken [103-124]: rod length – l = 30cm., radius of the cross-section of the rod -r = 2 cm, constant along the length of the rod, the elasticity modulus of the rod material – $E = 2 \cdot 10^6 kg/cm^2$, coefficient of thermal expansion $\alpha = 125 \cdot 10^{-7} (1/^{\circ}C)$, coefficient of thermal conductivity of the rod material – $K_{xxx} = 72(W/(cm^{\circ}C))$. Heat flux – $q(x) = -[3x + 10] (W/cm^2)$ is applied to the lateral surface of the rod by a linear law. Solving the system of linear algebraic equations (38) with the accepted initial data and using the property of the applied quadratic finite element, calculate the values of displacement, deformation, and stress for different (N=1) – one quadratic finite element (QFE), N=2-QFE, N=3-QFE, N=5-QFE, N=10-QFE), i.e., at 11, at 20, at 30, at 50, at a 100 equally spaced points and ten intervals between them. All calculated values and displacements, $\varepsilon_x, \varepsilon_T, \varepsilon_u, \sigma_x, \sigma_T, \sigma_u$ – elastic, temperature, and thermoelastic components of deformations and stresses were given in the corresponding tables (Table 1).

Table 1. Values and displacements, ε_x , ε_T , ε_u , σ_x , σ_T , σ_u – elastic, temperature, and thermoelastic components of deformations and stresses

Nodal points	\mathcal{E}_{x}	Nodal points	\mathcal{E}_T	Nodal points	ε_u
1	-0.0007335304	1	-0.0015142235	1	-0.0022477539
3	-0.0001168919	3	-0.0021320339	3	-0.0022489258
4	0.0001211149	4	-0.0023717985	4	-0.0022506836
7	0.0003945101	7	-0.0026457797	7	-0.0022512695
9	0.0000642736	9	-0.0023167151	9	-0.0022524414
10	-0.0002977196	10	-0.0019564796	10	-0.0022541992
Total:					-0.0225097656
Nodal points	$\sigma_{_{x}}$	Nodal points	$\sigma_{\scriptscriptstyle T}$	Nodal points	σ_u
1	-1467.0608108108	1	-3028.4470016892	1	-4495.5078125000
3	-233.7837837838	3	-3682.9761402027	3	-4497.8515625000
4	242.2297297297	4	-4743.5969172297	4	-4501.3671875000
7	789.0202702703	7	-5291.5593327703	7	-4502.5390625000
9	128.5472972973	9	-4633.4301097973	9	-4504.8828125000
10	-595.4391891892	10	-5083.5884712838	10	-4508.3984375000

Arithmetic mean:	-4501.9531250000

Note: $\sigma_u = -4501.953125$.



The values of 11 nodal displacements and the corresponding law of distribution of deformation and stress are presented in Figures 3-4:

Figure 3. Values of 11 nodal displacements along the length of the rod



Figure 4. Fields of distribution of the value of 11 nodal displacements corresponding to deformation and stress $(\varepsilon_x, \sigma_x, \sigma_T, \sigma)$ along the length of the rod

Similarly, the distribution field of the deformation value from the temperature field ε_T is presented in Figure 5



Figure 5. Values of 11 nodal deformations from the temperature field \mathcal{E}_T along the length of the rod

Analysing Table 1, it can be seen that the value of thermoelastic stress exceeds the exact $(\sigma = -4494.79 \ kg(f)/cm^2)$ solution by a maximum of 0.16%. In this regard, the considered rod is discretised with two (N=2) quadratic finite elements. At twenty fixed points, the values of elastic, temperature and thermoelastic components of deformations and stresses $-\varepsilon_x$, ε_T , ε_u , σ_x , σ_T , σ_u are given in Table 2, the corresponding fields of displacement, deformation and stress distribution in Figures 6-7, and the distribution field ε_T in the Figure 8.



Figure 6. Values of 20 nodal displacements along the length of the rod





Figure 7. Fields of distribution of the value of 20 nodal values corresponding to deformation and stress $(\varepsilon_x, \sigma_x, \sigma_T, \sigma)$ along the length of the rod



Figure 8. Values of 20 nodal deformations from the temperature field ε_T along the length of the rod Table 2. Values of elastic, temperature, and thermoelastic components of deformations and stresses

Nodal points	<i>E</i> _x	Nodal points	\mathcal{E}_{T}	Nodal points	ε _u
1	-0.0008192040	1	-0.0014283180	1	-0.0022475220
6	-0.0000507496	6	-0.0021972851	6	-0.0022480347
7	0.0000694257	7	-0.0023173871	7	-0.0022479614
13	0.0004061022	13	-0.0026545031	13	-0.0022484009
17	0.0001364126	17	-0.0023851064	17	-0.0022486938
20	-0.0004054054	20	-0.0018436547	20	-0.0022490601
Total:					-0.0449658203
Nodal points	σ_{x}	Nodal points	$\sigma_{_T}$	Nodal points	σ_u
1	-1638.4079391892	1	-2856.6360061233	1	-4495.0439453125
6	-101.4991554054	6	-4394.5701805321	6	-4496.0693359375
7	138.8513513514	7	-4634.7742029138	7	-4495.9228515625
13	812.2043918919	13	-5309.0061497044	13	-4496.8017578125
17	272.8251689189	17	-4770.2128642314	17	-4497.3876953125
18	-18.0743243243	18	-4479.7528241131	18	-4497.8271484375

20	-810.8108108108	20	-3687.3093063767	20	-4498.1201171875
Arithmeti	c mean:				-4496.5820312500

Note: $\sigma_{u} = -4496.58$.

Analysing Table 2, it can be seen that the largest deviation from the exact ($\sigma = -4494.79 \ kg(f)/cm^2$) solution is 0.04%. For engineering calculations, this accuracy is considered to be excellent, but, nevertheless, in order to reduce the error of the obtained numerical results, the considered rod is discretised with three (N=3) quadratic finite elements of the same length. As a result of solving the resolving systems of equations, the values of the sought variables at thirty fixed points are obtained and presented in Table 3, and the corresponding displacement field and the law of distribution of elastic, temperature, and thermoelastic components of deformations and stresses (ε_x , σ_x , σ_T , σ) along the length of the rod are given in Figures 9 -10, and the law of deformation distribution from the temperature field (ε_T) is given in Figure 11:



Figure 9. Values of 30 nodal displacements along the length of the rod



Figure 10. Fields of distribution of 30 nodal values corresponding to deformation and stress (ε_x , σ_x , σ_T , σ) along the length of the rod



Figure 11. Fields of distribution of values of 30 nodal deformations from the temperature field ε_T along the length of the rod

Nodal points	\mathcal{E}_{x}	Nodal points	\mathcal{E}_T	Nodal points	ε_u
1	-0.0008480512	1	-0.0013994061	1	-0.0022474573
9	-0.0000293387	9	-0.0022182922	9	-0.0022476309
10	0.0000506913	10	-0.0022983874	10	-0.0022476960
19	0.0004081144	19	-0.0026559623	19	-0.0022478479
26	0.0000686718	26	-0.0023167151	26	-0.0022480433
27	-0.0000356732	27	-0.0022123484	27	-0.0022480216
30	-0.0004441942	30	-0.0018039359	30	-0.0022481301
				Total:	-0.0674338108
Nodal points	$\sigma_{_{x}}$	Nodal points	$\sigma_{\scriptscriptstyle T}$	Nodal points	σ_u
1	-1696.1023523523	1	-2798.8122888512	1	-4494.9146412035
9	-58.6774274274	9	-4436.5844359983	9	-4495.2618634257
10	101.3826326326	10	-4596.7747043917	10	-4495.3920717591
19	816.2287287287	19	-5311.9246199322	19	-4495.6958912035
26	137.3435935936	26	-4633.4301097971	26	-4496.0865162035
27	-71.3463463463	27	-4424.6967670794	27	-4496.0431134257
30	-888.3883883883	30	-3607.8717389263	30	-4496.2601273146
Arithmetic mean:					-1195 5873812591

Table 3. The values of the sought variables at 30 fixed points

Note: $\sigma_{\mu} = -4495.58$.

In this case, it was revealed from the obtained numerical solutions that the maximum discrepancy between the σ_u value and the exact one $(\sigma_u = -4494.79 \, kg(f)/cm^2)$ is 0.017576%. Thus, it was found that with an increase in discrete finite elements, a decrease in errors is observed. If the considered rod is discretised with five (N=5) quadratic finite elements, then the obtained numerical results in Table 4 show that the maximum error in the value of the thermoelastic stress does not exceed 0.00641%.

Nodal points	<i>E</i> _x	Nodal points	\mathcal{E}_T	Nodal points	ε _u
1	-0.0008712331	1	-0.0013761864	1	-0.0022474195
15	-0.0000126642	15	-0.0022348210	15	-0.0022474852
16	0.0000353872	16	-0.0022828864	16	-0.0022474992
31	0.0004090574	31	-0.0026566176	31	-0.0022475602
44	0.0000083000	44	-0.0022559305	44	-0.0022476305
45	-0.0000579986	45	-0.0021896271	45	-0.0022476258
50	-0.0004762669	50	-0.0017713917	50	-0.0022476586
Total:					-0.1123769531
Nodal points	σ_x	Nodal points	σ_{T}	Nodal points	σ _u
1	-1742.4662162164	1	-2752.3728462840	1	-4494.8390625
15	-25.3283783784	15	-4469.6419341219	15	-4494.9703125
16	70.7743243243	16	-4565.7727618247	16	-4494.9984375
31	818.1148648650	31	-5313.2351773653	31	-4495.1203125
44	16.600000000	44	-4511.8609375003	44	-4495.2609375
45	-115.9972972973	45	-4379.2542652030	45	-4495.2515625
50	-952.5337837839	50	-3542.7834037165	50	-4495.3171875
Arithme	tic mean:			<u>.</u>	-4495.0781250004

Table 4. Numerical results of discretising a rod by five quadratic finite elements

Note: $\sigma_{\mu} = -4495.0781$.

The corresponding field of distribution of displacements along the length of the rod is presented in Figure 12.



Figure 12. Values of 50 nodal displacements along the length of the rod

This curve is based on the displacement values at 51 equidistant points. In this case, the distance between the points is 0.6 cm. It can be seen from this graph that approximately at the point with the coordinate x = 21.6 cm the displacement value will be zero. The corresponding strain and stress fields are presented in Figures 13-14.



Figure 13. Fields of distribution of 50 nodal values corresponding to deformation and stress (ε_x , σ_x , σ_T , σ) along the length of the rod



Figure 14. Fields of distribution of the value of 50 nodal deformations from the temperature field ε_T along the length of the rod

Then discretise the considered rod with ten (N=10) quadratic finite elements, then the obtained numerical value of the thermoelastic stress in Table 5 exceeds the exact ($\sigma_u = -4494.79 \, kg(f)/cm^2$) solution by 0.00163%.

Nodal points	E _x	Nodal points	\mathcal{E}_T	Nodal points	ε _u
1	-0.0008886803	1	-0.0013587217	1	-0.0022474021
30	-0.0000003670	30	-0.0022470532	30	-0.0022474202
31	0.0000236681	31	-0.0022710877	31	-0.0022474196
61	0.0004093758	61	-0.0026568131	61	-0.0022474372
87	0.0000241872	87	-0.0022716396	87	-0.0022474524
88	-0.0000075778	88	-0.0022398764	88	-0.0022474542
100	-0.0005009291	100	-0.0017465322	100	-0.0022474612
Total:					-0.2247431641
Nodal points	σ_{x}	Nodal points	$\sigma_{\scriptscriptstyle T}$	Nodal points	σ_u
1	-1777.3606418924	1	-2717.4434596715	1	-4494.8041015639
30	-0.7339527025	30	-4494.1064769865	30	-4494.8404296890
31	47.3361486489	31	-4542.1754064628	31	-4494.8392578140
61	818.7516891894	61	-5313.6261032534	61	-4494.8744140640
87	48.3743243241	87	-4543.2792071381	87	-4494.9048828140
88	-15.1555743246	88	-4479.7528241144	88	-4494.9083984390
100	-1001.8581081080	100	-3493.0643528303	100	-4494.9224609390
Arithmet	tic mean:		-4494.8632812515		

Table 5. Numerical value of thermoelastic stress

Note: $\sigma_{\mu} = -4494.86328$.

This accuracy in terms of thermal stability is very excellent. In this case, the corresponding field of displacement distribution is presented in Figure 15:



Figure 15. Values of 100 nodal displacements along the length of the rod

This figure shows that near the point x = 21.6 cm the displacement value will again be zero. The constructed deformation and stress fields are presented in Figures 16-17.



Figure 16. Fields of distribution of the value of 100 nodal displacements corresponding to deformation and stress (ε_{x} , σ_{x} , σ_{T} , σ) along the length of the rod



Figure 17. Fields of distribution of the value of one hundred nodal deformations from the temperature ε_T along the length of the rod

Thus, when calculating the thermal strength of rods of limited length clamped by two ends under action of the heat flux on the lateral surface changing along the coordinate, in order to obtain high-precision numerical results, it is necessary to discretise at least ten quadratic finite elements. After testing the developed mathematical model and the corresponding computational algorithm, the effect of the length of the rod on the thermo-stressed state was analysed. To do this, the values of the compressive force $R_{,(kg(f))}$ and the effective stress $\sigma_{,(kg(f)/cm^2)}$ were calculated for different values of the rod length. These results are shown in Table 6.

No.	L(cm)	R,(kg(f))	σ ,(kg(f)/cm ²)	%
1	30	-56454.58	-4494.79	100
2	27	-47446.29	-3769.61	83.86
3	24	-39522.13	-3146.66	70
4	21	-32893.79	-2618.93	58.26
5	18	-27272.95	-2179.375	48.48
6	15	-22871.3	-1820.96	40.5

Table 6. The effect of the length of the rod on the thermo-stressed state of the investigated rod

In addition, the thermal stress-strain state of the rod under consideration is influenced by the value of the heat transfer coefficient h, $(W/cm^2 \cdot C)$ between the material of the rod and the surrounding cross-sectional area of the clamped ends of the rod. This dependence on a specific example is shown in Table 7.

No.	$h,(W/cm^2 \cdot C)$	R,(kg(f))	$\sigma,(kg(f)/cm^2)$	%
1	10	-56454.58	-4494.79	100
2	9	-59332.916	-4723.958	105.1
3	8	-62930.83	-5010.41	111.47
4	7	-67556.72	-5378.72	119.66
5	6	-73724.583	-5869.79	130.59
6	5	-82359.583	-6557.29	145.88

Table 7. Influence of the heat transfer coefficient on the thermo-stressed state of the investigated rod

It should be noted that the thermo-stressed state of the investigated rod is also influenced by the value of the ambient temperature $(T_a, {}^0 C)$. These dependencies are shown in Table 8.

Table 8. Influence of ambient temperature on the thermo-stressed state of the investigated rod

No.	$(T_a, {}^0C)$	(R, kg(f))	$\left(\sigma, \frac{kg(f)}{cm^2}\right)$	%
1	40	-56454.58	-4494.79	100
2	35	-54884.58	-4369.79	97.22
3	30	-53314.58	-4244.79	94.438
4	25	-51744.58	-4119.79	91.657
5	20	-50174.58	-3994.79	88.876

4. Conclusion

Thus, a mathematical model and a corresponding computational algorithm for the numerical simulation of the thermo-stressed state of a rod clamped by two ends under influence of a heat flow on the lateral surface were developed. It has been proven that in order to obtain high-precision numerical results, it is necessary to discretise at least ten quadratic finite elements, then the calculation error does not exceed 0.00163%. When solving this problem, it was also found:

a) with a decrease in the length of the rod, the values of the compressive force (R) and the effective stress (σ) decrease in a nonlinear manner. In particular, with a decrease in the length of the rod by 10, 20, 30, 40 and 50%, the values of R and σ decrease by 16.14; 30; 41.74; 51.52 & 59.5%, respectively;

b) with a decrease in the value of the heat transfer coefficient in this example by 10, 20, 30, 40, and 50% leads to an increase in the values of the compressive force (R) and effective stress (σ), respectively, by 5.1; 11.47; 19.66; 30.59, and 45.88%;

c) with a decrease in the temperature value of the surrounding area of the cross-sections of the two clamped ends of the medium rod by 12.5; 25; 37.5, and 50% leads to a decrease in the values of the compressive force (R) and effective stress (σ), respectively, by 2.78; 5.562; 8.343, and 11.124%.

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