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ESTIMATION OF THE CERAMIC ADMIXTURE INFLUENCE ON THE POLYMERIZATION TEMPERATURE FOR SURGICAL CEMENT

This work concentrates on the mathematical analysis of the ceramic admixture influence on the temperature distribution into the polymerizable bone cement. It has been taken the simplified model, which consist in treatment the cement sample as a plate of the definite thickness. It has been determined the temperature field within the plate along the thickness of the sample, during the polymerization process. It was found that Al_2O_3 admixture added into the bone cement first of all affects on the change of maximal polymerazation temperature through the increase of the temperature condictivity coefficient a for PMMA-Al_2O_3 composite. Assuming that the coefficient a for the composite is twice higher than for PMMA, the calculated maximal temperature for the polymerizing system decreases to about 30%.

1. INTRODUCTION

The bone cements are the most often used biomaterials for endoprostheses of joints in orthopedia and traumatology. The bone cement is the very important component of the artificial joint, which has an influence on its durability. After polymerization process the surgical cement acts as an element connected the prosthesis with bone [3]. The bone cements for the most part belong to the group of polymer-matrix composites. The chemical composition of the cements, the materials kind, method of theirs preparation and polymerization process in the bone, affect on the cements properties [5,6,13,14].

There are numerous types of bone cements currently produced in the world, which are self-polymerizing acrylic masses. They are formed in the course of operation from the mixture of powder polymer and liquid monomer. PMMA (polymethyl methacrylate) is usually used as a polymer component, whereas MMA (methyl methacrylate) as a monomer component.

Polymerization is an exothermal process. In this way the temperature of formed bone cement is raised higher. From medical point of view high temperature of cement polymerization, which is significantly higher than the temperature of protein coagulation is unfavourable leading to central necrosis [5,7,14].

During the surgical cement implantation it is in contact directly with the metal prosthesis at the initial room temperature 19 ^{0}C on the one hand, and with the living bone at the human temperature about 37 ^{0}C on the other hand. The influence of this two kinds of boundary conditions on the polymerization temperature have been presented in the previous works [1,2]. It has been used

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the Palacos R cement, that has been polymerized inside a heated metal mould. The investigations have been shown, that the initial temperature of the mould has significant influence upon the temperature of the cement polymerization. Into the mould at the initial temperature 19 ^{0}C the polymerization temperature was about 40 ^{0}C, when by initial temperature 37 ^{0}C the maximum polymerization temperature reached 109 ^{0}C.

The work [2] attempts at modification of chemical composition of commonly used PMMA based surgical cements, which should lower their polymerization temperature. The investigations have been shown, that into the mould at the initial temperature 37 ^{0}C the maximal polymerization temperature of the Palacos R cement with Al_2O_3 powder admixture (13% in volume fraction) decreases by about 3,6%.

This work concentrates on the mathematical analysis of the ceramic admixture influence on the temperature distribution into the polymerizable bone cement.

2. PROBLEM FORMULATION

The analysis of the temperature distribution into the polymerizable surgical cement has been performed. It has been taken the simplified model, which consists in treatment the cement sample as a plate by the definite thickness. It has been determined the temperature field into the plate by thickness equal 2b, for the first kind boundary conditions [4,12], in the form of the function of the change of temperature in course of time:

$$T (x = \pm b) = f (t) \tag{1}$$

It has been found the initial condition in the form:

$$T (t = 0) = F (x) \tag{2}$$

It has been written the equation of the thermal conductivity in case, when it is assumed an influence of the volumetric heat source:

$$\partial T / \partial t = a \, \nabla^2 T + q_v / (c \, \rho) \tag{3}$$

where:

   a – thermal diffusion coefficient (temperature conductivity coefficient),
   c – specific heat,
   ρ – density,
   T – temperature,
   t – time,
q_v in this case is the capacity of the heat source related to the volume unit:

$$q_v = \dot{q} \, \rho \tag{4}$$

where:

$\dot{q}$ - capacity of the heat source related to the mass unit, variable in course of time.
On this ground it has been gotten:

$$\partial T / \partial t = a \nabla^2 T + \dot{q} / c \qquad (5)$$

Subsequently it is possible to write:

$$\dot{q} / c = D(t), \qquad (6)$$

therefore:

$$\partial T / \partial t = a \nabla^2 T + D(t) \qquad (7)$$

We search for the solution of the equation (7) in the form:

$$T = f(t) + u(x, t) \qquad (8)$$

In the equation (5) the time derivative is defined by the formula:

$$\partial T / \partial t = \dot{f}(t) + \partial u / \partial t, \qquad (9)$$

however second x derivative of temperature is defined by formula:

$$\partial^2 T / \partial x^2 = \partial^2 u / \partial x^2 \qquad (10)$$

On this ground it has been gotten:

$$\partial u / \partial t = a \, \partial^2 u / \partial x^2 - \dot{f}(t) + D(t) \qquad (11)$$

The searched function *u* ought to perform the following conditions:

$$\begin{cases} u(x = \pm b) = 0 \\ u(t = 0) = F(x) - F(0) \end{cases} \qquad (12)$$

It has been taken, that it is possible to present the solution of the equation (11) in the form of the following series [8,12]:

$$u = \sum_{i=1}^{n} A_i(t) \cos \delta_i (x/b), \qquad (13)$$

where:

$$\delta_i = [(2i-1)/2] \cdot \pi \; (i=1,2,...)$$

Subsequently it has been taken, that the temperature of the external surface is constant. Then it has been gotten:

$$\dot{f}(t) = 0, f(t) = T_p, \tag{14}$$

where T_p is the temperature of the surface.
In this case it is possible to write the thermal conduction equation in the form:

$$\partial u / \partial t = a \, \partial^2 u / \partial t^2 + D(t) \tag{15}$$

Presenting $D(t)$ in the form of the series, it has been gotten:

$$D(t) = \sum_{i=1}^{n} B_i \cos\delta_i (x/b) \tag{16}$$

It is possible to write the coefficients B_i in the following form:

$$B_i = [\int_{-b}^{b} D(t) \cos\delta_i (x/b) \, dx] / [\int_{-b}^{b} \cos^2\delta_i (x/b) \, dx] \tag{17}$$

After carrying out integration it has been calculated:

$$B_i = [2(-1)^{i+1} D(t)] / \delta_i \tag{18}$$

After the replacement of the equation (16) and (13) to the equation (15) it has been gotten:

$$\sum_{i=1}^{n} \dot{A}_i(t) \cos\delta_i (x/b) = -a/b^2 \sum_{i=1}^{n} A_i(t) \delta_i^2 \cos\delta_i (x/b) + \sum_{i=1}^{n} B_i \cos\delta_i (x/b) \tag{19}$$

This equation can be satisfied, when:

$$\dot{A}_i(t) + (a/b^2) \delta_i^2 A_i(t) = B_i \tag{20}$$

The solution of the equation (20) is described by following formula:

$$A_i(t) = C_i \exp(-\delta_i^2 \, at/b^2) + \exp(-\delta_i^2 \, at/b^2) \int_0^t \exp(\delta_i^2 \, at/b^2) B_i \, dt \tag{21}$$

It is possible to evaluate the constants C_i from the initial condition ($t=0$):

$$F(x) - f(0) = \sum_{i=1}^{n} C_i \cos\delta_i \, (x/b) \qquad (22)$$

Taking into consideration the equation (14) it has been found:

$$F(x) - T_p = \sum_{i=1}^{n} C_i \cos\delta_i \, (x/b) \qquad (23)$$

For the series, written this way, it has been evaluated the coefficients C_i from the following formula:

$$C_i = \{ \int_{-b}^{b} [F(x) - T_p] \cos\delta_i \, (x/b)dx \} / \{ \int_{-b}^{b} \cos^2 \delta_i \, (x/b)dx \} \qquad (24)$$

Subsequently on the assumption, that the initial temperature is constant in the plate cross-section: $F(x)=T_0$, after carrying out integration, it has been gotten:

$$C_i = [\, 2(-1)^{i+1} \, (T_0 - T_p) \,] / \delta_i \qquad (25)$$

After the replacement of the equation (25) and (18) to the equation (21) it has been gotten:

$$A_i(t) = exp(- \delta_i^2 \, at/b^2) \cdot [\, 2(-1)^{i+1}(T_0 - T_p)]/ \delta_i +$$

$$+\{[2(-1)^{i+1}]/ \delta_i \}exp(- \delta_i^2 \, at/b^2) \cdot \int_{o}^{t} \, exp(\delta_i^2 \, at/b^2)D(t)dt \qquad (26)$$

Replacement of the value $D(t)$ to equation (26) is the next stage of the calculation..
Taking the following form of $D(t)$:

$$D(t) = K_q \, exp(-\varphi t), \qquad (27)$$

where: K_q, φ – coefficients,
it has been written:

$$A_i(t) = exp(- \delta_i^2 \, at/b^2) \, [2(-1)^{i+1}(T_0 - T_p)]/ \delta_i +$$

$$+\{[2(-1)^{i+1}]/ \delta_i \}exp(- \delta_i^2 \, at/b^2) \cdot [K_q/(\delta_i^2 \, a/b^2 - \varphi)] \, [exp(\delta_i^2 \, at/b^2 - \varphi t)-1] \qquad (28)$$

On this ground:

$$u = \sum_{i=1}^{n} A_i \, (t) \cos\delta_i \, (x/b) \; and$$

$$T = T_p + \sum_{i=1}^{n} A_i \ (t) \ cos\delta_i \ (x/b) \qquad (29)$$

3. RESULTS AND DISCUSSION

For the purpose of modelling the temperature distribution along the thickness of the sample, during the polymerization process, it has been taken the thermal condition equation in the form of the equation (5):

$$\partial T / \partial t = a \nabla^2 T + \dot{q} /c,$$

It has been evaluated the capacity of the heat source, variable in course of time. For this purpose it has been taken, that the heat of the polymerization of MMA to PMMA equals 60 kJ/mol. Because the mass number of PMMA amount to 100 g (5 particles of carbon at 12g, 2 particles of oxygen at 1g, 8 particles of hydrogen at 1g), therefore the heat of polymerization amount to:

$$q = 60 \ kJ/mol \cdot (1 \ mol/100 \ g) = 0,6 \ kJ/g = 600 \ kJ/kg.$$

It has been taken, that the heat of polymerization q is emited in the most part during the first period of the polymerization process. At that time the temperature increases. Then the temperature decreases as a result of the heat exchange with an environment. For the bone cement time of the rapid increase amount to from 8 to 12 minutes.

It has been assumed, that it is possible to write $\dot{q}/c$ in the form:

$$\dot{q} /c = D(t) = K_q \ exp(-\varphi t) \qquad (30)$$

where:

K_q (K/min) – coefficient,
φ (1/min) – coefficient,
t (min) – time.

It has been selected the coefficient K_q and φ on the ground of the experimental results. It has been taken the total polymerization time amounted to $t_p \approx 25$ minutes.

After carrying out integration of the equation (30) on coordinate t, it has been gotten:

$$\int_{0}^{t_p} K_q \ exp(-\varphi t)dt = - (K_q/\varphi) \ [exp(-\varphi t_p) - 1] \qquad (31)$$

Therefore:

$$q /c = (K_q/\varphi) \ [1 - exp(-\varphi t_p)] \qquad (32)$$

Taking the following values:

$t_p = 25$ min,
$\varphi = 0,11$ 1/min,
$q = 600$ kJ/kg,
$c = 2,2$ kJ/(kg K),

it has been evaluated the value K_q:

$$K_q \approx q \, \varphi / c = 30 \, K/min.$$

Subsequently it has been calculated change of the polymerization temperature in course of time, along the thickness of the sample, taking the value of the temperature conductivity coefficient amounted to $a = 1 \times 10^{-3}$ m^2/h $\approx 1 \times 10^{-5}$ m^2/min. The values range of the coefficient a, given in the literature [10,11] for the polymers amount to from $0,1 \times 10^{-3}$ m^2/h to $1,5 \times 10^{-3}$ m^2/h. The results of the calculations are been presented in Fig.1.
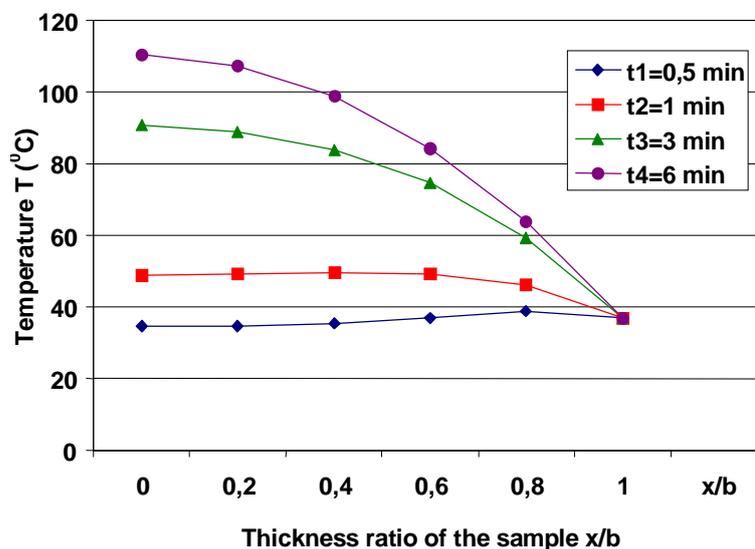

Fig.1. Temperature distributions in function of thickness ratio of the sample for various times

The addition of the Al$_2$O$_3$ powder to PMMA based surgical cement have an effect on the change of the polymerization heat q, density ρ (on the ground the formula: $\dot{q} = q_v / \rho$) as well as on the change of the temperature condictivity coefficient a for the forming composite.

It was found that Al$_2$O$_3$ admixture added into the bone cement (in quantities 5% in volume fraction) first of all influence on the change of maximal polymerization temperature through the increase of the coefficient a for PMMA- Al$_2$O$_3$ composite. Because the value of the temperature condictivity coefficient a for Al$_2$O$_3$ is about 100-times higher than for PMMA and it amount to 32,4 $\times 10^{-3}$ m^2/h [9,10].

Assuming, that the coefficient a for the composite is twice higher than for PMMA, so it amount to 2×10^{-5} m^2/min, the calculated maximal temperature for the polymerizing system decreases to about 30% (Fig.2 and Fig.3).
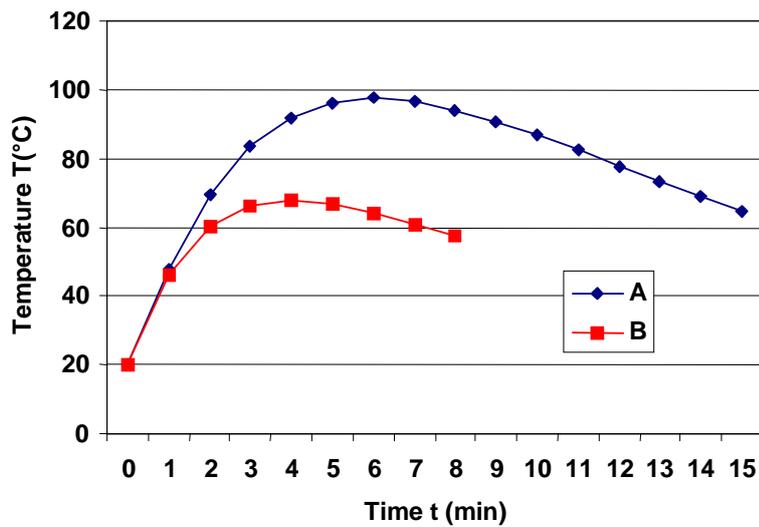
Fig.2. Change of maximal polymerization temperature in course of time for surgical cement without admixtures (A) and with Al_2O_3 admixtures (B) into a mould model at the temperature 19°C
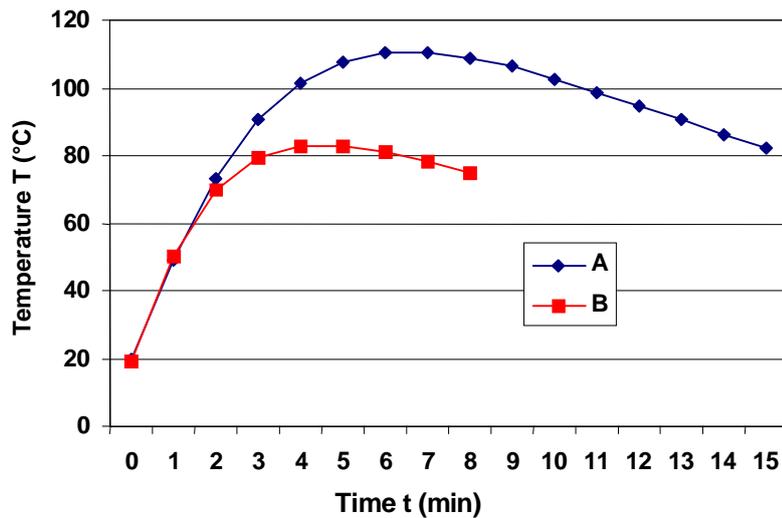

Fig.3. Change of maximal polymerization temperature in course of time for surgical cement without admixtures (A) and with Al_2O_3 admixtures (B) into a mould model at the temperature 37°C

It has been stated, that it is possible to decrease the polymerization temperature of the surgical cement by on addition of ceramic particles and that it is possible to model an influence of the particles volume fraction on the polymerization temperature by the way, which has been shown in the paper.

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