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SOLVING APPLIED PROBLEMS OF NONLINEAR MATHEMATICAL PROGRAMMING

The article presents mathematical models for embryo division technologies using laser spots and laser segments. It should be noted that laser segment division is used when there are a large number of blastomeres in the embryo, otherwise laser spot division technology is used. These mathematical models are non-local boundary value problems for unsteady partial differential heat conduction equations. Despite the three-layer structure of the embryo (pellucid zone, perivitelline space, and blastomere cell layer), it is appropriate to consider it as a homogeneous body when calculating the temperature of the laser action on the embryo. Averaging the thermal conductivity coefficients for the embryo layers is acceptable due to their insignificant differences in these layers.

After analyzing existing numerical methods used to solve boundary value problems, the authors propose using the Galerkin method. This means that the solution to the heat conduction differential equation must be sought in the form of a Fourier series, whose unknown coefficients are calculated taking into account the boundary and edge conditions in the mathematical models used in the calculations. The authors guarantee the thermal stability (viability) of the embryo by controlling the heating at the point of laser focus on the embryo and in the adjacent, nearest areas of the embryo, since it is at these points that coagulation processes in the embryo can occur during laser exposure. This control is possible by taking into account the viability temperature of the embryo when setting the boundary conditions in the specified boundary value problems. It should be noted that the research in this article belongs to the theory of analysis and synthesis of complex systems, and the considered problem of calculating the damaging temperature of laser exposure on the embryo belongs to the applied problems of nonlinear mathematical programming.

Keywords: *computational mathematical models, Galerkin method, complex systems, thermal stability of the embryo.*

Formulation of the problem. Processes in technical and biotechnological systems containing local, concentrated, mobile sources of influence, including local sources of scanned laser radiation, are described using nonlocal boundary value problems for systems of partial differential equations. However, using the traditional theory of the existence and uniqueness of solutions to boundary value problems with differential equations, it is not always possible to prove the correctness of boundary value problems. In this case, to obtain and justify the condition of correctness of boundary value problems, it is advisable to apply the theory of pseudodifferential operators over the space of generalized functions.

The article proposes computational mathematical models for technologies that affect the embryo with a laser source in the form of a spot and a segment in order to reduce the trauma to blastomere cells during subsequent transplantation. From a thermophysical point of view, an embryo is a spherical microbiological object with different thermal conductivity coefficients for its layers (the pellucid zone, the perivitelline space, and the blastomeres). However, due to the insignificant difference in thermal conductivity coefficients for the layers, for the purpose of numerical calculations, it is possible to transition to a homogeneous medium with averaging of thermal conductivity coefficients. The blastomeres are asymmetrically distributed within the embryo, and their number varies. In addition, it should be noted that the embryo is placed in a cannula with a nutrient medium, which is maintained at a temperature $37\ {}^0C$ that ensures the viability of the embryo.

The embryo is exposed to a pulsed laser source in the form of a spot if the number of blastomeres is small, or a segment if the number of blastomeres is large (18, 36, or 64 cells). To ensure the viability of the separated parts of the embryo, careful temperature control is necessary at the points in the embryo closest to the center of the laser exposure. In addition, it should be noted that after a brief pulsed laser exposure, the electromagnetic exposure ceases and the heat flow from the more heated area of the embryo flows into the separated parts of the embryo.

Analysis of recent research and publications. In order to improve the accuracy and speed of automation in the design of complex systems, mathematical models were developed in monograph [1] and implemented using numerical methods. Numerical methods are proposed for solving boundary value problems with differential equations when the spatial coordinates belong to regions of arbitrary spatial shape [2, 3]. At the same time, articles [2, 3] take into account that the boundary of the regions can be not only a rectangular surface but also a cylindrical or spherical surface. The authors of articles [4, 5] have constructed computational mathematical models under conditions of uncertainty in the input data for differential equations, the right-hand side of which takes into account impulse perturbations.

The results of article [6] are devoted to the design and implementation of an automated autonomous power supply and life support system for general use to increase the resistance of a residential building's cyber-physical system to external factors. The authors of article [7] obtained conditions for the existence and uniqueness of solutions for a linear differential equation of infinite order with an arbitrary commutative domain. The methods proposed in article [8] for solving second-order differential equations with partial derivatives of hyperbolic type allowed its authors to calculate the consumption of composite materials for individual technological processes. The proposed physical and mathematical models for calculating the thermal heating modes of a two-layer cylinder and creating protective coatings for the surfaces of devices subjected to thermal stress [9–11]. The authors of article [12] solved the transport problem of a motor train movement along a track, taking into account the terrain relief.

Task statement. Build mathematical models for laser spot and laser segment embryo division technologies.

Outline of the main material of the study. In the case of using laser spot embryo division technology, the boundary condition for the laser exposure process will be as follows:

$$\delta(x,y,z)\frac{\partial T(x,y,z,t)}{\partial t}=\lambda\Delta T(x,y,z,t)+P(x,y,z,t), \quad (1)$$

where $\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$ – Laplace operator;
T – temperature;
x,y,z – spatial coordinates;
t – exposure time;
$P(x,y,z,t)$ – a function characterizing the distribution of the laser energy source and represented as:

$$P(x,y,z,t)=\begin{cases}P(x,y,z,t),\ if\ (x,y,z)\in L,\ t\in[0;\tau];\\ 0,\ if\ (x,y,z)\notin L,\ t\notin[0;\tau],\end{cases} \quad (2)$$

L – laser source range;
τ – pulse source duration.

Desired temperature distribution $T(x,y,z,t)$ from the equation (1) must satisfy the initial and boundary conditions, respectively:

$$T(x,y,z,t)\big|_{t=0}=T(x,y,z), \quad (3)$$

$$\left[\frac{\partial T(x,y,z,t)}{\partial v_{01}}+h_{01}(x,y,z)T(x,y,z,t)\right]\Bigg|_{(x,y,z)\in\Gamma_{01}}=T_{01}(t), \quad (4)$$

where h_{01} – heat transfer coefficient;
v_{01} – normal direction Γ_{01}.

In addition, boundary conditions are imposed on the target function at the interfaces between media, for example, on the outer shell of the embryo and the nutrient medium:

$$\lambda_3\frac{\partial T(x,y,z,t)}{\partial v_3}=\lambda_4\frac{\partial T(x,y,z,t)}{\partial v_4}, \quad (5)$$

$$\lim_{(x,y,z)\to(x^*,y^*,z^*)}T(x,y,z,t)=T(x^*,y^*,z^*,t), \quad (6)$$

where $\left(x^*, y^*, z^*\right)$ – limit values, permissible values of spatial coordinates.

Similarly, conditions of the form (5)–(6) are formed for other contiguous regions: the embryo shell (pellucid zone)–perivitelline space, blastomeres–perivitelline space [13].

To solve equation (1) with the corresponding initial and boundary conditions, it is advisable to apply, for example, a combination of Laplace transformation and one of the variational methods: Ritz, Galerkin, or the Fourier method of separating variables. However, the complexity of the structure of the thermophysical system under consideration (embryo–laser radiation) is such that it is not possible to expect to obtain a solution in a few minutes on modern computers. Such requirements are related to ensuring the viability of the embryo. In addition, embryos presented for division have significant differences, both in the number of blastomeres (2, 4, 8, 16, 32, 64 cells) and in their location within the embryo. All this complicates the process of calculating the temperature fields of embryos in the biotechnological process and requires significant costs. Therefore, based on the specifics of the embryo and the analysis of boundary conditions (1)–(6), it is reasonable to propose a way to reduce the task of calculating the temperature field to a simpler one, ensuring accuracy consistent with the accuracy of the working parameters of the technical means that ensure embryo division by a laser beam [14–16].

The most significant feature of mathematical modeling of laser exposure to the embryo is that the exposure carrier can be circular, spherical, extended, and narrow, with its dimensions (radius or width) hundreds of times the diameter of the embryo. The thermal conductivity coefficients of the embryo layers do not differ significantly, which means that the embryo can be represented as a homogeneous body with an average thermal conductivity coefficient. When considering the thermal regime of the embryo, the nutrient medium of the embryo with a temperature $37\ {}^0C$ can be excluded and the corresponding conditions can be set at the outer boundary of the embryo. In this case, during laser exposure to the embryo, the center of the embryo will be the most heated.

Thus, the first approximate physical model of the interaction of laser radiation with an embryo can be a model of a spherical body with uniform thermal conductivity, which is exposed to a spherical laser source moving at a certain speed and dividing the embryo into two parts. This physical model of an embryo exposed to laser radiation is necessary for precise laser cutting of the embryo. This is because, in the early stages of embryo development (2, 4, 8 blastomeres), it is necessary to ensure that the trajectory of the source affects as few blastomeres as possible. This technology of laser embryo division, based on the use of a local mobile laser source, is called laser spot division technology.

Let us consider the first physical model of embryo division by laser cutting, which takes into account the spherical shape of the embryo and the average values of the thermal conductivity coefficients of points in the embryo layers. The unsteady temperature field of a spherical body with uniform thermal conductivity and radius *R*, containing in the center (the most loaded temperature regime) a discrete pulse source with a radius $T = T\left(x, y, z, t\right)$, is described in a spherical coordinate system by the following parabolic equation:

$$\frac{\partial T\left(r,t\right)}{\partial t} - a\left(\frac{\partial^2 T\left(r,t\right)}{\partial r^2} + \frac{2}{r}\cdot\frac{\partial T\left(r,t\right)}{\partial r}\right) = \frac{q\left(r,t\right)}{\rho c}, \quad (7)$$

where $T\left(r,t\right)$ – excessive temperature;
r – radial coordinate;
t – time;
$a = \dfrac{\lambda}{\rho c}$ – thermal temperature-conductivity coefficient;
λ – thermal conductivity coefficient;
ρ – density coefficient;
c – heat capacity coefficient;
$q\left(r,t\right)$ – density of the laser source.

Suppose that ideal heat exchange with the environment is specified on the spherical surface of the body. In this case, the following initial conditions apply to equation (7):

$$\begin{cases} T\left(r,t\right)\big|_{t=t_0} = 0; \\ T\left(r,t\right)\big|_{r=R} = 0 \end{cases} \quad (8)$$

and specific heat flux conditions (4).

Note that the formulation of the boundary value problem (7)–(8), i.e., without taking temperature into account $37\ {}^0C$ embryo's nutrient medium, is possible due to the linearity of the boundary value problem operator. This means that the result of solving boundary value problem (7)–(8) will be the distribution of excess temperature generated only by the source, which can then be easily converted to temperature by taking into account the temperature at the embryo–nutrient medium boundary.

Using Galerkin's method, we will seek a solution to boundary value problem (7)–(8) in the form of a series expansion:

$$T\left(r,t\right) = \sum_{n=1}^{\infty} b_n\left(t\right)\frac{1}{r}\sin\frac{\pi n r}{R}. \quad (9)$$

To search for unknown functions by time $b_n(t)$ substitute $T(r,t)$ from (9) into equation (7) and obtain the differential equations:

$$b_n^t + B_n b_n = \frac{2}{R\rho c}\int_0^R rq(r,t)\sin\frac{n\pi r}{R}dr\,, \quad (10)$$

where $B_n = \frac{an^2\pi^2}{R^2}$;

b_n^t – the index at the top indicates differentiation by t.

Let us use the zero initial conditions (8) and, solving equation (10), determine $b_n(t)$. After substitution $b_n(t)$ in solution (9) of boundary value problem (7)–(8), we obtain the final distribution of the excess temperature field in the form:

$$T(r,t) = \frac{2}{r\pi\rho c}\sum_{n=1}^{\infty}\frac{1}{n}\sin\left(\frac{n\pi r}{R}\right)F_n(r,t), \quad (11)$$

where $F_n(r,t)$ has the following form:

$$F_n(r,t) = \frac{2}{R\rho c}\int_0^t e^{-A_n(t-u)}\int_0^R rq(r,u)\sin\left(\frac{n\pi r}{R}\right)drdu\,. \quad (12)$$

In equation (12) q – this is the density distribution of the laser source, which we will define as a pulse with a duration of *h* his actions.

For a temperature field mode that is «loaded» when an extended laser radiation source passes through the center of a spherical body, the temperature field distribution is not centrally symmetric, as was the case in the first physical model. Therefore, a spherical coordinate system is unacceptable.

The obtained analytical, albeit approximate, solution of the corresponding boundary value problem is necessary for solving the synthesis problem associated with determining the power values and geometric parameters of the laser source affecting the embryo. The numerical representation of the temperature field does not allow for the effective solution of the synthesis problem.

The second approximate physical model could be a spherical body with uniform thermal conductivity, divided by a laser source in the form of a segment whose maximum length is equal to the diameter of the embryo. Such a laser spot scan into a segment can be achieved using optical devices. Note that, as in the case of the first physical model, the moment when the source passes through the center of the spherical body will be the most «loaded» in terms of the level of temperature field creation. This is due to the fact that a constant temperature of the nutrient medium is maintained at the outer boundary of the embryo, equal to $37\ {}^0C$.

This laser embryo division technology is acceptable when the embryo has reached the stage of 16, 32, and 64 blastomeres. This means that the number of blastomeres is large and this technology ensures that there are enough undamaged blastomere cells in the embryo segments. At the same time, the absence of blocks for setting and controlling the trajectory of the laser beam, as in the case of the above model of local laser spot exposure, significantly reduces equipment costs and ensures the thermal stability (viability) of the divided parts of the embryo. This technology of laser embryo division, based on the expansion of the laser spot into a segment, is called laser segment division technology.

Considering that the width of the laser source is several hundred times smaller than the diameter of the embryo, the length of the source is equal to the diameter of the embryo when the source passes through the center of the sphere, and the temperature at the outer boundary of the embryo is maintained at $37\ {}^0C$ nutrient medium, the embryo area closest to the source will be the most «loaded» in terms of temperature. The temperature field created by the laser in the embryo is described by the following parabolic equation:

$$c\rho\frac{\partial T}{\partial t} = \lambda\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right), \quad (13)$$

where c – heat capacity coefficient;

ρ – density coefficient;

$T = T(x,y,z,t)$ – excessive temperature;

x, y, z – spatial coordinates;

t – time;

λ – thermal conductivity coefficient.

The following source model is assumed: flat, surface-mounted with heat dissipation density $g_0(x,y,t)$:

$$g_0(x,y,t) = \begin{cases} \frac{P_0(t)}{a_x b_y}, (x,y)\in S,\, t\in[t_0;t_n]; \\ 0, (x,y)\notin S,\, t\notin[t_0;t_n], \end{cases} \quad (14)$$

where $P_0(t)$ – heat release capacity of the source over time;

a_x, b_y, h – source dimensions;

S – area occupied by the source carrier;

$[t_0;t_n]$ – source duration.

Boundary conditions at the top of the domain:

$$\left.\frac{\partial T}{\partial z}\right|_{z=0} = \psi_0(x,y,t), \quad (15)$$

were

$$\psi_0(x,y,t) = \frac{g_0(x,y,t)}{\lambda}. \quad (16)$$

Condition on the outer edge ($z = h$) is set as follows:

$$T\left(x,y,z,t\right)\Big|_{t=h}=T_k\left(x,y,t\right). \quad (17)$$

Initial condition related to the moment in time $t=0$:

$$T\left(x,y,z,t\right)\Big|_{t=0}=T_0\left(x,y,t\right). \quad (18)$$

At the lateral boundary of the domain, the boundary conditions are:

$$\left.\frac{\partial T}{\partial x}\right|_{\substack{x=0,\\ x=A_x}}=\left.\frac{\partial T}{\partial y}\right|_{\substack{y=0,\\ y=A_y}}=0. \quad (19)$$

For the formulated mathematical model (13) – (19), the temperature field is a heating process, which can be represented as follows:

$$T_{heat}\left(x,y,z,t\right)=U_{heat}\left(x,y,z,t\right)+\left(z-h\right)\psi_0\left(x,y,t\right), \quad (20)$$

were

$$U_{heat}=\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\sum_{r=0}^{\infty}V_{nmr}\left(t\right)\cos\frac{n\pi x}{A_x}\times\cos\frac{m\pi y}{A_y}\cdot\cos\frac{\left(2r+1\right)\pi z}{2h}, \quad (21)$$

V_{nmr} – can be represented as Fourier series.

Thus, the above method for calculating the temperature field in an embryo when exposed to a laser beam is one of the main methods for the numerical implementation of boundary value problems describing the technology of embryo division by a laser beam, with the aim of finding the optimal technical parameters of laser emitters.

Conclusions. The mathematical models for the process of laser exposure to the embryo developed in this article are based on the theory of analysis and synthesis of complex systems with local, mobile sources of physical fields. Based on the analysis of the structural features of the embryo and the specifics of the assumptions made, it was possible to construct mathematical models for embryo division technologies using a laser spot and a laser segment. These features allowed us to conclude that, depending on the stage of embryo development, when constructing mathematical models of the process of laser exposure to the embryo, it is necessary to analyze these two technologies separately.

The authors show that these mathematical models are based on nonlocal boundary value problems for differential heat conduction equations with boundary and boundary conditions. Despite the fact that the embryo is a three-layer microbiological object, due to the chemical composition of its layers, it is advisable to switch to a homogeneous medium with averaged values of thermal conductivity coefficients for the layers in order to perform numerical calculations of the resulting (excess) temperature field and subsequent optimization of the control technical parameters of laser emitters, it is advisable to switch to a homogeneous medium with averaged values of thermal conductivity coefficients for the layers. Such models are necessary for analyzing the dynamics of temperature fields in an embryo divided by a laser beam in order to obtain viable parts of a microbiological object (embryo). Note that the task of calculating the excess temperature field for a multilayer system belongs to a special type of nonlinear mathematical programming problems.

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Левкін Д.А., Завгородній О.І., Левкін А.В., Чалий І.В. РОЗВ'ЯЗАННЯ ПРИКЛАДНИХ ЗАДАЧ НЕЛІНІЙНОГО МАТЕМАТИЧНОГО ПРОГРАМУВАННЯ

В статті побудовані розрахункові математичні моделі для технологій ділення ембріона лазерним п'ятном і лазерним відрізком. Відзначимо, що ділення лазерним відрізком застосовують коли велика кількість клітин бластомірів в ембріоні, в іншому ж випадку застосовують технологію ділення лазерним п'ятном. Зазначені розрахункові математичні моделі – це нелокальні крайові задачі для нестаціонарних диференціальних рівнянь теплопровідності в частинних похідних. Незважаючи на тришарову (зона пелюцида, перивительований простір і шар клітин бластомірів) будову ембріона, для розрахунку температури лазерної дії на ембріон доречно його розглянути в якості однорідного тіла. Усереднення коефіцієнтів теплопровідності для шарів ембріона припустимо через незначну їх відмінність в цих шарах.

Проаналізувавши існуючі чисельні методи, які застосовуються для розв'язання крайових задач, автори пропонують застосувати метод Галеркіна. Це означає, що розв'язок диференціального рівняння теплопровідності потрібно шукати у виді ряда Фур'є, невідомі коефіцієнти якого обчислюють, врахувавши граничні і крайові умови в розрахункових математичних моделях. Автори гарантують теплову стійкість (життєздатність) ембріона за рахунок контроля нагріву в місці фокусування лазерної дії на ембріоні і в прилеглих, найближчих областях в ембріоні, адже саме в цих точках можуть відбуватися процеси коагуляції в ембріоні під час лазерної дії. Зазначений контроль можливий за рахунок врахування температури життєздатності ембріона під час завдання граничних умов в зазначених крайових задачах. Потрібно відзначити, що дослідження цієї статті належать до теорії аналізу і синтезу складних систем, а розглянута задача розрахунку збиткової температури лазерної дії на ембріон – до прикладних задач нелінійного математичного програмування.

Ключові слова: *розрахункові математичні моделі, метод Галеркіна, складні системи, теплова стійкість ембріона.*

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