A new computer code for calculation of radiation and heat fields in laser irradiated tissues

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ABSTRACT

A non-stationary two-dimensional computer code for modelling of radiation and heat transport in heterogeneous biological tissues irradiated with laser is presented. Radiation transport is considered in the kinetic model, radiation transport equation is solved by the Monte Carlo method. Heat transport is considered in the heat conduction model, the heat equation is solved by a combination of Galerkin and the finite element methods. The code has passed a number of tests including comparisons with analytical solutions, numerical calculations of other authors, and with experimental results. The code can be used for working out and designing of laser surgical and therapeutic procedures. As well it can be used in inverse problem of experimental determination of optical and thermal parameters of biological tissues.

Keywords: laser, radiation, temperature, the Monte Carlo method, the finite element method, tissue.

1. INTRODUCTION

The information about radiation and heat fields in laser irradiated biological tissues is important for laser surgery, photo and thermotherapy. It is very desirable for institute of such speciality to have a computer code for evaluation of such fields. A few created codes[1-5] do not cover the demands of the institutes both in respect of accuracy and availability.

In this work we present our code for calculation of non-stationary two-dimensional distributions of different radiation characteristics and temperature in heterogeneous turbid media (biological tissue, first of all), irradiated with laser. The calculations are performed in two stages: radiation and heat ones. On the first stage we use the kinetic model of light transport and the Monte Carlo method, on the second stage - the heat equation model and a combination of the finite elements and Galerkin's methods.

2. MODEL OF MEDIUM

We use a two-dimensional axial symmetry model of a medium. The heterogeneous medium is represented as a cylinder consisting of homogeneous ring zones of rectangular section (fig. 1) with their optical and thermophysical parameters. Such geometry is in good agreement with cylindrical symmetry of laser beams and allows sufficiently adequate modelling of radiation and heat effects in a lot of real tissues.

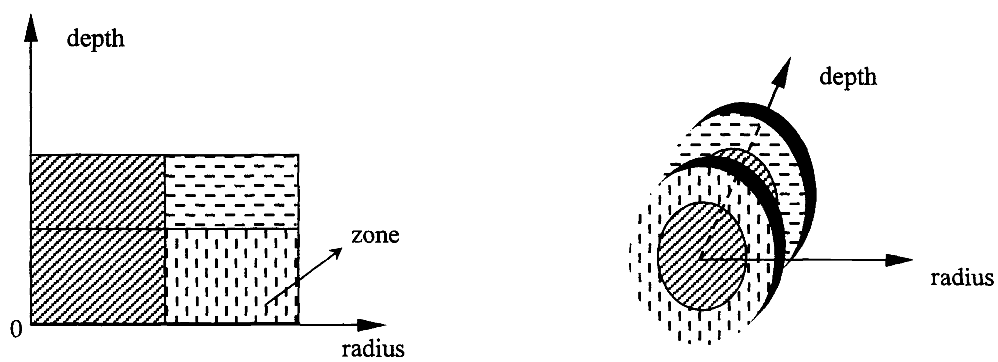

Fig. 1. Model of heterogeneous medium.

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3. RADIATION TRANSPORT MODEL

We use the kinetic model, one of the most adequate models of optical radiation transport in scattering and absorbing media. In this model the radiation transport is interpreted as the process of multiple scattering of photons on randomly distributed inclusions of medium. The basic characteristic of radiation field is the differential energy flux density (differential intensity) $I(\boldsymbol{r}, \Omega, t)$ in a point $\boldsymbol{r}$, in a direction Ω, at a time t. It satisfies to the radiation transport equation, quasi-stationary in our case (photon time life in medium is negligible, t is a parameter):

$$\Omega \nabla I(\mathrm{r},\Omega,t)+\mu(\mathrm{r},t)\, I(\mathrm{r},\Omega,t)-\int \mu_s(\mathrm{r},t)\, p(\mathrm{r},\Omega\cdot\Omega')\, I(\mathrm{r},\Omega',t)\, d\Omega'=S(\mathrm{r},\Omega,t), \tag{1}$$

where $\mu \equiv \mu_a + \mu_s$, μ_s, μ_a are coefficients (macroscopic cross sections) of interaction, scattering and absorption, resp., p is the indicatrix of scattering (distribution of photon scattering angle $\theta = \arccos(\Omega',\Omega)$, S is the source function (differential power density of radiation emitted by the source). As the indicatrix we use the Heney-Grinstein function, traditional for biooptics:

$$p(\cos\theta)=\frac{1-g^2}{4\pi\left(1-2g\cos\theta+g^2\right)^{3/2}} \tag{2}$$

where g is the anisotropy factor (the average cosine of scattering angle). As boundary conditions we accept those following Fresnel's formulas for light reflection and refraction on border of zones with different refractive indexes n. So, the data necessary for radiation transport modelling are the source function S and medium optical parameters μ_a, μ_s, g, n for each zone.

4. HEAT TRANSPORT MODEL

The main ways of heat transport inside any object are heat conduction, convection and thermal radiation transport. The latter is negligible in the temperature range to be considered. We take into account the thermal conduction in medium and the convection in boundary conditions. This model approximately describes thermal processes in tissues with capillary blood flow, which is taken into account in transport coefficients. The mathematical representation of the model is the non-stationary heat equation for each zone V_i (open domain in $\boldsymbol{R}^3$) of the medium $V=\sum_i V_i$ (over all the zones) with the heat sources from laser radiation, calculated on the radiation stage, and initial and boundary conditions which allow zone-zone and medium-environment interactions:

$$c\rho\frac{\partial T}{\partial t}=k\Delta T+Q \tag{3}$$

$$T\big|_{t=0}=T_0 \tag{4}$$

$$(\theta\, k\boldsymbol{n}\cdot\nabla T+\beta T-\psi)\big|_{\Gamma}=0 \tag{5}$$

$$\left(k_A\boldsymbol{n}_{AB}\cdot\nabla T_A-k_B\boldsymbol{n}_{AB}\cdot\nabla T_B\right)\big|_{\Gamma_{AB}}=0 \tag{6}$$

$$(T_A-T_B)\big|_{\Gamma_{AB}}=0 \tag{7}$$

$$Q(\boldsymbol{r},t)=\mu_a(\boldsymbol{r},t)\int_{4\pi} I(\boldsymbol{r},\boldsymbol{\Omega},t)\,d\boldsymbol{\Omega}$$

where $T=T(\boldsymbol{r},t)$ is the medium temperature to be calculated in a point $\boldsymbol{r}$ at an instant t; $c,\rho,\ k$ are specific heat capacity, mass density and thermal conductivity, resp., (they are constant over a zone and possibly are dependent on time); $Q=Q(\boldsymbol{r},t)$ is the heat source, the power density of laser radiation absorbed by medium in a point $\boldsymbol{r}$ at an instant t; Γ is the outside (medium-environment) border of medium V; Γ_{AB} is the border between adjacent zones A and B; $\boldsymbol{n}$, $\boldsymbol{n}_{AB}$ is the outside normal to Γ and A to B normal to Γ_{AB} ; T_A, k_A, T_B, k_B are the temperatures and the thermal conductivities in zones A and B; θ, β, ψ are parameters determining a kind of outside boundary conditions. By choosing these parameters we take into account the following physical conditions on the outside border Γ:

- conservation of temperature ($\theta = 0$, $\beta = 1$, ψ is the temperature); (8)
- conservation of thermal flow ($\theta = 1$, $\beta = 0$, ψ is the flow); (9)
- heat exchange under the Newton law ($\theta = 1$, $-\beta$ is the heat-transfer coefficient, ψ/β is the environment temperature near boundary Γ. (10)

The conditions (6,7) provide the physical requirements on the inside borders: continuity of temperature and heat current density.

5. CALCULATION OF RADIATION FIELDS

Solution of the radiation transport equation (1) is carried out by the analog Monte Carlo method[6]. The photon trajectories are simulated in full accordance with the given source function S, optical parameters μ_a, μ_s and indicatrix (2) with the given factor g. When a photon achieves a boundary of a zone (inside or outside), it undergoes either reflection or diffraction according to Fresnel's formulas. For estimation of space distribution of absorbed power density (heat source Q) we divide each zone of medium into small ring cells of rectangular section (fig. 2), and during simulation of photon trajectories we determine absorbed energy in the each cell. Absorbed power density in a cell is accepted a constant equal to average value of the density over the cell. In addition to Q we can estimate other radiation characteristics: space and angular distributions of flux and current density of photon energy, reflection and transmission characteristics and other functionals of differential intensity I.

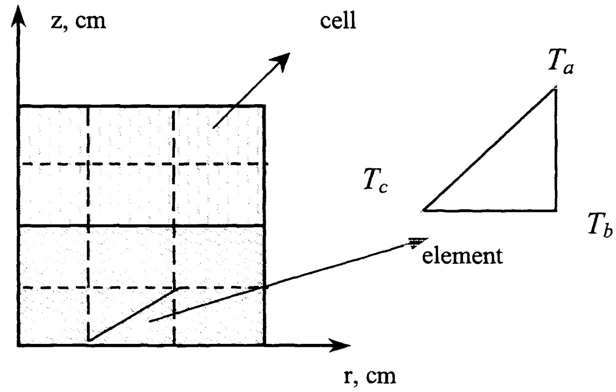


Fig. 2. Discretization of 2-zone domain.

6. CALCULATION OF HEAT FIELDS

The non-stationary temperature field $T(\mathbf{r},t)$, the solution of eq. (3), is calculated step by step in time, beginning from initial condition (4). Let τ_1 be an instant time when the temperature field $T_1(\mathbf{r})=T(\mathbf{r},\tau_1)$ have already been determined. For determination of the field $T_2(\mathbf{r})=T(\mathbf{r},\tau_2)$ at the next instant $\tau_2 = \tau_1 + \tau$, $(\tau > 0)$ approximate the time dependence of the field $T(\mathbf{r},t)$, $\mathbf{r} \in V$, on interval (τ_1, τ_2) by the linear function:

$$T(\mathbf{r},t) \approx T_{1,2}(\mathbf{r},t) \equiv N_1(t)T_1(\mathbf{r}) + N_2(t)T_2(\mathbf{r}), \tag{11}$$

where $N_1(t)$, $N_2(t)$ are the linearly independent basic functions:

$$N_1(t) = \frac{\tau_2 - t}{\tau}, \quad N_2(t) = \frac{t - \tau_1}{\tau}$$

Since the dependence $T_{1,2}$ is not correct absolutely the residual of eq. (3)

$$\varepsilon(\mathbf{r},t) = \frac{\partial T_{1,2}}{\partial t} - \frac{k}{c\rho}\Delta T_{1,2} - \frac{Q}{c\rho}, \quad t \in (\tau_1, \tau_2), \mathbf{r} \in V,$$

is not equal to zero at any field T_2. For determination of T_2 we minimize the residual in sense of Galerkin's method: we find T_2 from the orthogonality condition:

$$\int_{\tau_1}^{\tau_2} N_2(t)\varepsilon(\boldsymbol{r},t)\,dt = 0 \quad \text{for all point } \boldsymbol{r} \text{ of the medium } V.$$

As a result we obtain the following equation for determination of the field T_2

$$\tilde{k}\Delta T - \alpha T + \tilde{Q} + \frac{\tilde{k}}{2}\Delta T_1 = 0 \ , \tag{12}$$

where $T \equiv T_2$, $\tilde{k} = \frac{\tau}{3}k$, $\tilde{Q} = \frac{c\rho}{2}T_1 + \frac{\tau}{2}Q$, $\alpha = \frac{c\rho}{2}$. The same boundary conditions (5)-(7) must be used.

So, we reduce a non-stationary problem to sequence of stationary problems. For solving the equation (12) with the boundary conditions (5)-(7) we use the finite element method[7]. It is based on minimization of a variational functional for the corresponding problem. The functional for the problem (12), (5)-(7) with boundary conditions (8) has the form:

$$\chi = \sum_i \int_{V_i} \frac{1}{2}\left[\tilde{k}(\nabla T)^2 - 2\tilde{Q}T + \alpha T^2 + \tilde{k}\nabla T \cdot \nabla T_1\right] dV, \tag{13}$$

where the summation is taken over all zones of the medium V. The minimization must be performed in the class of functions $T(\boldsymbol{r})$ continuous over the all zones and its boundaries under conditions (7), (8): $T|_\Gamma$ is fixed (no variation).

The functional for the same problem under boundary condition (9), (10) has another form:

$$\chi = \sum_i \int_{V_i} \frac{1}{2}\left[\tilde{k}(\nabla T)^2 - 2\tilde{Q}T + \alpha T^2 + \tilde{k}\nabla T \cdot \nabla T_1\right] dV - \\ - \int_\Gamma \left(\frac{\beta}{2}T^2 - T\psi + \frac{\tilde{k}}{2}T\boldsymbol{n}\cdot\nabla T_1\right) d\Gamma \tag{14}$$

The continuity of T over zones and boundaries must be provided at minimization.

For minimizaton of the functionals the domain V is divided on finite number of ring elements with triangular cross sections. We use the same system of cells as in calculation of the heat source function Q in the radiation stage (fig. 2). The cell sizes are a subject of choice. They must be small enough to provide a sufficient approximation of both functions Q and T. Within each of the elements the unknown temperature T is represented by the linear combination of temperatures T_a, T_b, T_c in nodes $\boldsymbol{r}_a$, $\boldsymbol{r}_b$, $\boldsymbol{r}_c$ of the element:

$$T(\boldsymbol{r}) = \varphi_a(\boldsymbol{r})T_a + \varphi_b(\boldsymbol{r})T_b + \varphi_c(\boldsymbol{r})T_c, \tag{15}$$

$\varphi_i = \frac{1}{2S}(a_{1i} + a_{2i}r + a_{3i}z)$, $a_{1i}=r_j z_k - r_k z_j$, $a_{2i}=z_j - z_k$, $a_{3i}=r_k - r_j$, $i, j, k = a, b, c$,

where (r, z) are cylindrical coordinates of vector $\boldsymbol{r}$, S is the area of element cross section.

Using the approximation (15) in the functionals (13), (14) varying them under the indicated conditions we obtain the final system of the linear equations:

$$\boldsymbol{K}\,\boldsymbol{T} = \boldsymbol{F}$$

where $\boldsymbol{T}$ is a column of temperatures in the element nodes at the end of considered time step, the values to be calculated;

$\boldsymbol{K}$ is a matrix dependent on node coordinates, on the medium parameters k, c, ρ, on the duration of time step τ, and on the heat-transfer coefficients if the boundary condition (10) is considered;

$\boldsymbol{F}$ is a column dependent on heat source function in the elements, on the known node temperatures at the beginning of the time step, on parameters k, c, ρ, τ, on the node coordinate, and on the parameter ψ in boundary conditions.

7. RESULTS

The described algorithm is realized as a computer code in FORTRAN. The code passed a number of tests including comparison of our results with analytical solutions, numerical calculations made with other codes, and with experimental data. Some of these comparisons are presented on fig. 3-6.

The fig.3 shows the excellent agreement between our and MCML[8] calculations of the main radiation characteristic (absorbed power density) in a typical laser geometry.

The fig. 4 demonstrates the full agreement between calculated and analytical temperatures in a simple non-stationary heat problem.

We had a good agreement in more complicated problem, including non-stationary two-dimensional transport both radiation and heat (fig.5). We compared our results with data calculated with the LITT code[2]. The data is given by authors of LITT in private communication.

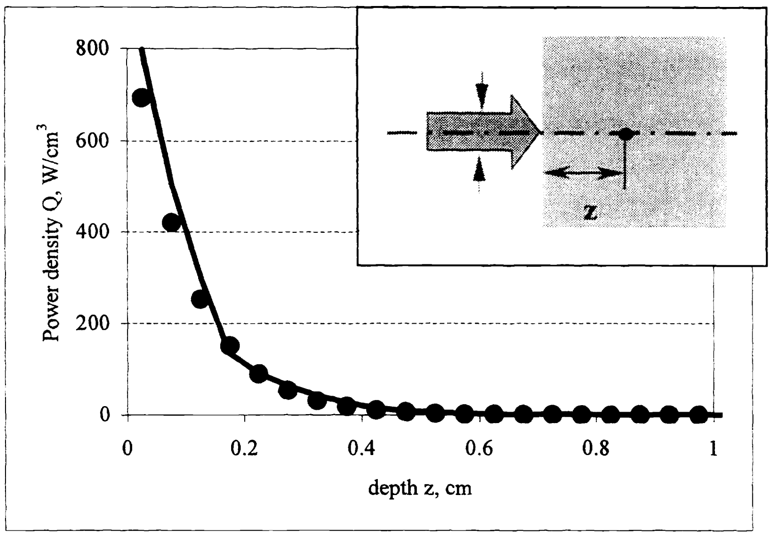


Fig. 3. Absorbed power density of laser radiation in semi-infinite homogenous medium at different depths on the beam axis. Beam profile is cylindrical flat, diameter d=0.1cm, power equals to 1 W. Medium parameters are: μa= 10.0 cm^{-1}, μs= 1.0 cm^{-1}, g=0.9, n=1.5. Solid line shows our data, points are data calculated with the MCML code.

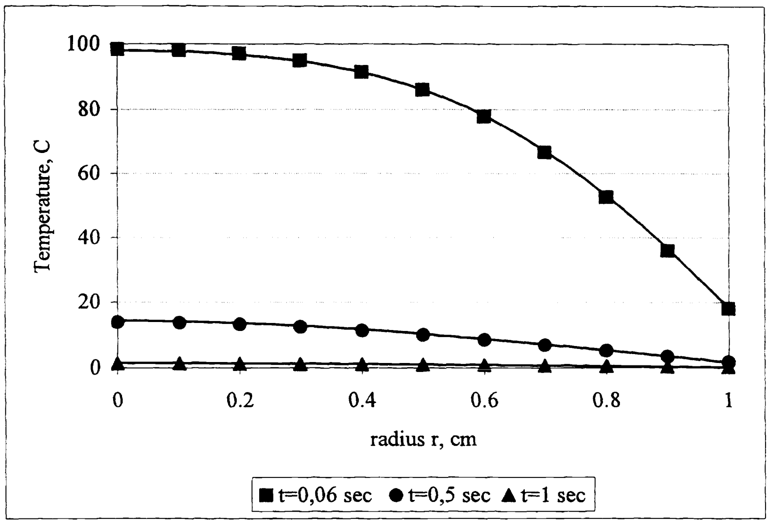


Fig.4. Temperature at 3 instants t within an infinite homogenous cylinder of radius 1 cm placed in a medium of fixed temperature 0 °C. The heat-transfer coefficient equals to 10 W/cm^2·K. Substance parameters are: ρ=1g/cm^3, k=1 W/cm·K, c=1 J/g·K. Solid lines are the data calculated by our code, points are analytical data.

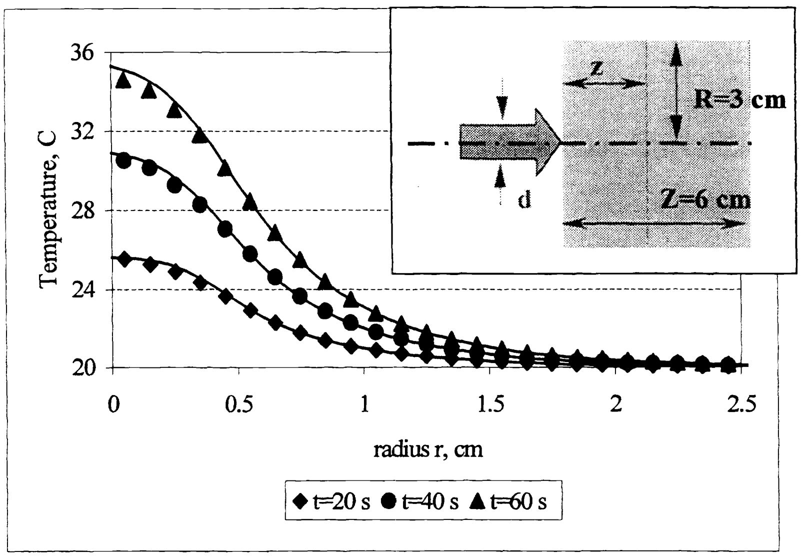
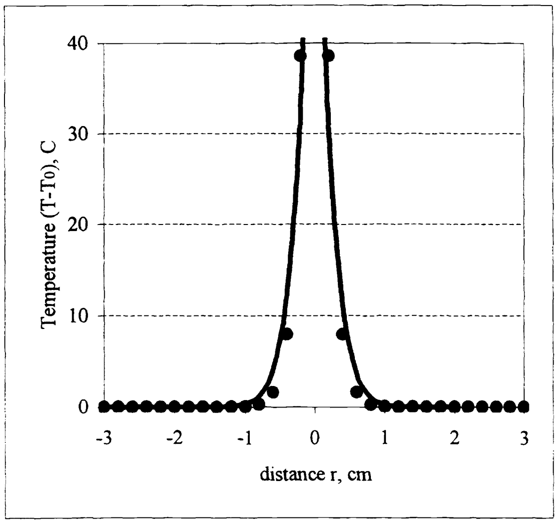


Fig.5. Temperature at 3 instant times within finite homogenous cylinder at the plane z=0.55 cm, irradiated by cylindrical monodirectional laser beam. Profile of the beam is flat, diameter d=1cm, power equals to 5 W. The frontal cylinder surface (z=0) is isolated (no heat exchange), the rest surfaces are in a contact with a medium of fixed temperature 20 °C; heat-transfer coefficient equals to 1.0 W/cm^2·K. At initial instant t=0 the temperature over whole cylinder was a constant (20 °C). Substance parameters are: μa= 0.2 cm^{-1}, μs= 50.0 cm^{-1}, g=0.95, n=1.4, k=0.0048 W/(cm·K), ρ=1.075 g/cm^3, c=3.4882 J/(g·K). Solid lines are our calculations, points are calculations by the LITT code.

On fig. 6 we compare our numerical calculations with analytical and experimental data in a heat problem with a point heat source in infinite homogeneous medium. Measurements were performed with an original setup created by us for determination of the termophysical parameters: the specific heat capacity c and the thermal conductivity k. A potato of size about 10 cm, was used as the medium in the experiment. An electric heat source of size about 1 mm was placed into the centre of the potato, temperature was measured by mean of thermocouples of sizes 0.3 mm. The comparisons allowed us to determine the range of source-detector distance and the time interval where the finiteness of medium and source is not significant, and it is possible to use analytical solutions in the inverse problem (determination of c and k).



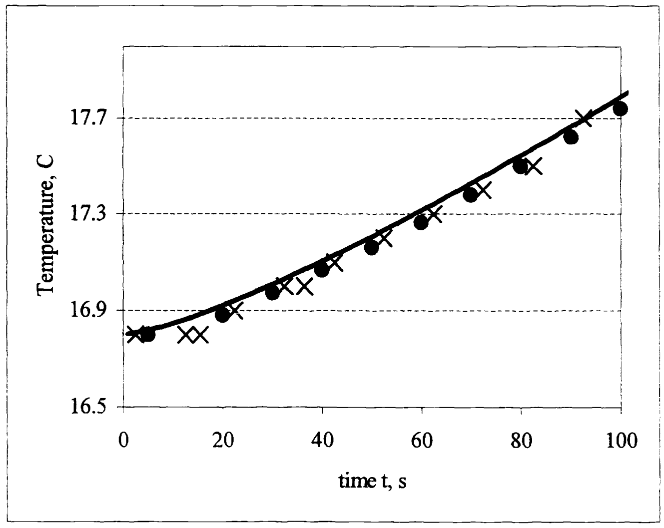


Fig. 6. Temperature in infinite homogeneous medium from a point heat source of fixed power 0.5 W. The left figure is the dependence on source distance r at an instant t=15 s, the right one is the dependence on time at a fixed source distance r=0.85 cm. At initial instant t=0 the temperature over whole medium was a constant (T_0= 16.8 °C). Substance is a potato with the parameters ρ=1.1 g/cm^3, k=0.01 W/(cm·K), c=4.4 J/(g·K) (our own measurements). Solid lines are calculations, points are analytical solution, crosses are our experimental data (see text).

Some capabilities of our code are illustrated with Fig. 7, 8 where modelling results of thermal action of He-Ne laser on skin in two operating modes (continuous and pulse) are presented. The modelling of such sort allows us not only to find out the parameters of laser irradiation as a preliminary, but to study, justify, and may be reveal the effects of laser action. In particular, the presented calculations demonstrate the effect of heat localisation for the pulse operating mode in comparison with the continuous. It is interesting to note that the localisation is not accompanied by temperature increase (see fig.8).

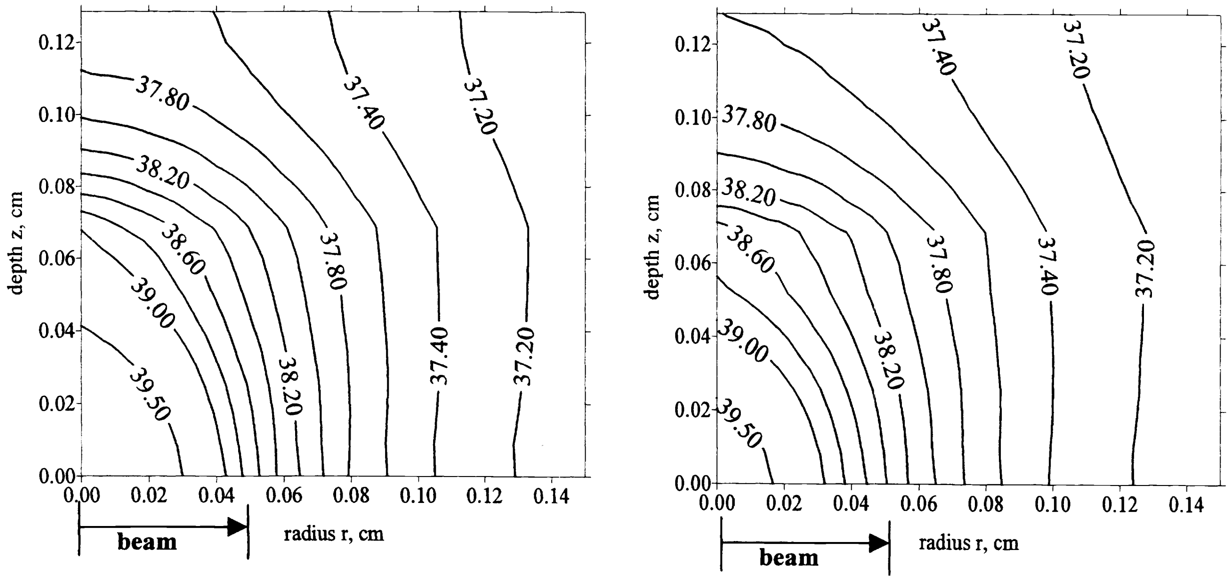


Fig. 7. Isotherms in skin irradiated by cylindrical monodirectional beam of He-Ne laser for the continuous (the left) and the pulse (the right) operating modes at an instant 1.5 s after the laser on. Profile of the beam is flat, diameter equals to 0.1cm, average power 25 mW at both modes, pulse duration 0.02 s, frequency 10 Hz. Initial temperature equals 37 °C. Heat exchange between the skin and environment is left out of account. Skin model is 4 layers one with the following parameters[5]:

Layer	thickness, mm	μ_a, 1/cm	μ_s, 1/cm	g	n	k, 10^{-3} W/cm·K	ρ, g/cm^3	c, J/(g·K)
1.Epidermis	0.065	4.3	107.0	0.79	1.5	2.66	1.6	3.7
2. Derma	0.565	2.7	187.0	0.82	1.4	4.98	1.0	3.2
3. Blood	0.09	25.0	400.0	0.98	1.35	5.30	1.0	3.6
4. Derma	0.565	2.7	187.0	0.82	1.4	4.98	1.0	3.2

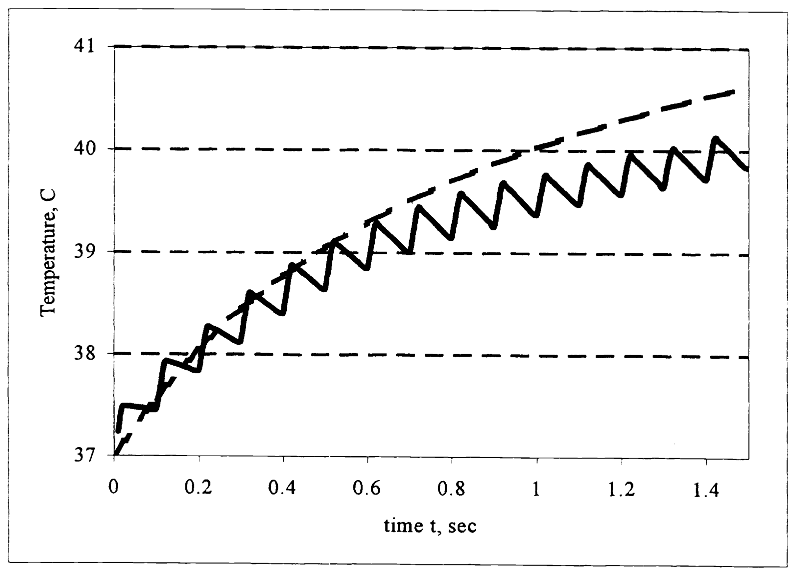


Fig.8. Time dependence of temperature at a point on frontal surface of skin on beam axis in the same problem as in fig.7. The continuous mode results are shown by dotted line, the pulse one by solid.

8. CONCLUSION

There are many cases where the presented code is useful. It allows simulation of laser surgical operations and laser procedures of thermotherapy and biostimulation, solving direct and inverse problems of the optics and the thermophysics of biological tissues. In the next code version we are going to use the accelerated local Monte Carlo estimate of radiation characteristics[9]. This estimate allows us to calculate more accurately the strongly non-uniform radiation fields. We also intend to involve more adequate models of blood flow and to apply other modifications.

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