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Modification of the multigroup approach for the monoenergetic electron beam propagation problem

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The paper presents a numerical solution to the problem of target heating by a monoenergetic electron beam. In the one-dimensional case, the solutions of the Boltzmann equation in the multigroup approximation, the solution without energy group splitting (exact), and a method called hybrid, which can be considered intermediate between the multigroup approximation and the exact solution for a monoenergetic beam, are analyzed and compared in detail. The considered numerical methods for electron transport in matter were implemented as a separate module into hydrodynamic code 3DLINE. The simulations were performed in the two-dimensional case, with analysis of the target heating characteristics by a monoenergetic electron beam, comparing the multigroup method and the hybrid approach, which in the monoenergetic case coincides with the exact solution.

Keywords: Boltzmann transport equation, fast electrons, hydrodynamics numerical calculations.

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Introduction

Numerical solution of a problem of heat transfer in matter in presence of electron flow propagating therein is of specific academic interest due to its complexity. This problem also arises as a subproblem in some other physical processes related to matter heating. Experimental studies show that heat transfer by fast electrons shall be taken into account in problems of inertial confinement fusion, fast ignition [1–3] and a warm dense matter [4,5]. One of the problems requiring taking into account contribution of electron transport to matter heating, is a problem of target laser irradiation. At relatively low intensities of laser radiation (not higher than $10^{14}\,\mathrm{W/cm^2}$) energy distribution of heated particles is Maxwellian, therefore, it is not required to separately take into account contribution to heating by electron transport. With such parameters, plasma dynamics is simulated using a hydrodynamic approach. A process of fast electrons generation becomes substantial, in case the following condition for laser radiation parameters is fulfilled $I\lambda^2 > 10^{14}\,\mathrm{W}\cdot\mu\mathrm{m}^2/\mathrm{cm}^2$, where I is intensity of laser radiation and λ is a wavelength of laser radiation [6]. At such parameters, the electron energy distribution differs strongly from the Maxwellian one. Due to high energy of the particles their transport is essentially non-local [7]. As a result, the hydrodynamic approach becomes inapplicable in an unchanged form.

Conditionally, methods of plasma dynamics simulation can be divided into three large groups: kinetic, hydrodynamic and hybrid methods [8]. The kinetic methods are the most fruitful in terms of a number of effects to be resolved during numerical modeling with correct numerical parameters. But it can be difficult to use them due to large space and time ranges in problems dealing with laser-matter interaction [9]. The exclusively hydrodynamic approach becomes inapplicable as said above. Therefore, the mixed approach is attractive for using in a class of problems requiring kinetic description of heat transfer by electrons [10,11]. Computations are simplified using modifications of a particle-in-cell method (PIC), for example, with a simplified model of dense plasma description, which is based on Ohm's law [9]. Various methods are used to solve the Vlasov–Fokker–Plank equations [12,13]. Improved hydrodynamic codes are extensively used, in which the electron transport problem is solved by the kinetic methods, for example, hybrid calculations using the PIC methods [14,15] with a built-in module for solving the electron transport equation [16,17]. Propagation of electrons in matter can be described using the Monte Carlo method [18], iteration methods [19] as well as a multi-group approximation.

The multi-group numerical method performs a transition from a continuous energy spectrum to a discrete one, at which the energy range is divided into a certain number of intervals (energy groups) [20]. The multi-group method is widely applied to neutron transport problems [21] and there are various modifications of this method [22,23]. This method being suitable for solving transport equations of particles, including electrons [24,25], is used in the hydrodynamic codes [26,27]. A numerical specific feature of the multi-group approximation is smearing of an absorption peak with an insufficient number of energy groups. Im-

provement of accuracy of energy input calculation requires an increase of the number of the groups, thereby increasing computational complexity.

The present study considers the most effective way of numerically taking into account heat transfer by electrons in matter as exemplified by irradiating a target with a monoenergetic electron beam based on the multi-group method or its variety. The modification of the classic multi-group approach is formulated to make it possible to obtain a solution using only one group that coincides with the exact solution for a case of the monoenergetic particle beam. Unlike the multi-group approximation, it does not exhibit „smearing“ of the absorption peak in the monoenergetic beam problems. This method does not require tracing of trajectories of separate electrons and can be easily generalized for taking into account reflective boundary conditions as well as presence of scattering in a multi-dimensional case. The present study compares the classic and the improved multi-group method and estimates influence of the numerical methods on physical process description.

In Section 1 of the present study we formulate parameters of the problem and an approximation, in which it is solved. In Section 2 we discuss a solution for the monoenergetic case without scattering. Sections 3 and 4 contain discussion the multi-group method and analysis of its convergence. Sections 5 and 6 are dedicated to considering the hybrid method In Section 7 we comparatively analyze the hybrid and the multi-group method in two-dimensional hydrodynamic calculation for the problem of interaction of the monoenergetic electron flow with matter in the approximation without scattering.

1. Basic physical approximations

Let us consider evolution of a distribution function of fast electrons $f(t, \mathbf{x}, \Omega, E)$, where t is time, $\mathbf{x}$ is a coordinate, Ω is a direction and E is energy. We neglect interaction with an average field [28] and take into account only collisions with electrons of a medium of the density n. In this case, the Boltzmann equation takes the following form

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{x}} = -v(E)n\sigma(E)f$$
$$+\int d\Omega' \int dE' v(E')n\sigma(E')\chi(E', \Omega'\cdot\Omega)g(E', E)f(t, \mathbf{x}, E', \Omega'). \quad (1)$$

Here, $\mathbf{v} = v(E)\Omega$ is an electron velocity, n is concentration of scatterers, $\sigma(E)$ is a full scattering cross-section, $\sigma(E')g(E', E)$ is a differential scattering cross-section $E' \to E$, $\chi(E', \Omega\cdot\Omega')$ is a scattering indicatrix. For g and χ , the following normalization conditions are met

$$\int g(E', E)dE = 1, \quad \int \chi(E', \Omega\cdot\Omega')d\Omega = 1.$$

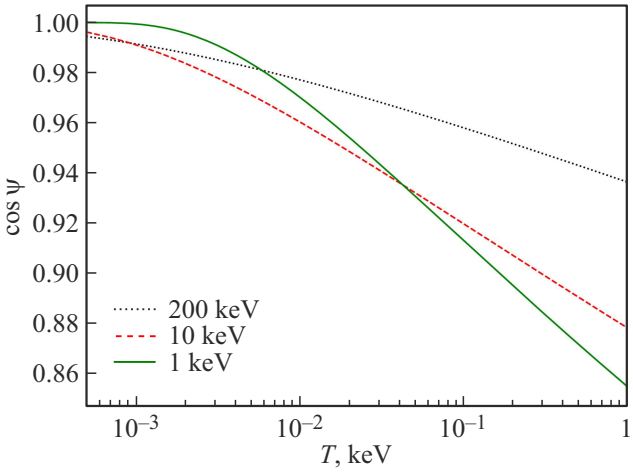

Figure 1. Dependence of the average cosines of the scattering angle to full stop on the medium temperature for the various values of the electron energy.

A ratio of a characteristic electron flight time to full stop to a characteristic time scale of hydrodynamics can be evaluated as a ratio of the electron velocity to the speed of sound in matter. Then, if energy of incident electrons exceeds greatly the temperature of the substance, the electron energy absorption process can be regarded in a quasi-stationary approximation resulting in neglection of the term $\partial/\partial t$.

Influence of scattering on the process of transport of electrons with the energy ε in the substance with the density ρ_{gcc}, the ion average charge Z and the temperature T_{keV} can be estimated via a value of an average cosines of the scattering angle, which is calculated by a formula of the study [29]:

$$\langle\cos\Psi\rangle = \sqrt{1 - \exp\left(-\frac{\pi^2}{4Z}\frac{f_{st}}{f_{sc}}\gamma_b\right)},$$
$$f_{st} = 11.2 - 0.5\ln\left(\frac{Z\rho_{gcc}}{A}\frac{\gamma_b}{(\gamma_b - 1)^2}\right), \quad (2)$$
$$f_{sc} = 6.7 - 0.5\ln\left(\frac{Z\rho_{gcc}}{AT_{keV}}\frac{1}{(\gamma_b - 1)\gamma_b}\right),$$
$$\gamma_b = 1 + \frac{\varepsilon}{mc^2}.$$

Let us consider absorption of the electrons of the energy of 200 keV in cold aluminum with the density of 2.678 g/cm^3 and the average ion charge $Z = 2.5$. The dependence of the average cosines of the scattering angle on the temperature is plotted in Fig. 1 according to the formulas (2). As can be seen from the graph, scattering becomes substantial only at the final stage of deceleration when the electron energy is comparable to the medium temperature. Thus, when the temperature of the substance is below 10 eV, the average scattering cosines when the beam losses the energy from 200 to 1 keV is below 0.02 and distribution of 99.5 % of the absorbed energy is described

with accuracy of no worse than 2% when assuming that there is no scattering, i.e. $\chi(\Omega \cdot \Omega') = \delta(\Omega - \Omega')$.

In this case, the various directions in the equation (1) become independent and the problem can be considered in the one-dimensional quasi-stationary approximation for the function $f(x, E)$:

$$v \frac{\partial}{\partial x} f(x, E) = -\sigma(E) n v f(x, E) + \int dE' \sigma(E') n v(E') f(x, E') g(E', E). \quad (3)$$

Let us consider variation of the energy flux density

$$W(x) = \int v(E) f(x, E) E dE,$$

$$\frac{d}{dx} W(x) = -n \int \sigma(E) v(E) f(x, E) \big(E - \varepsilon(E)\big) dE.$$

Here,

$$\varepsilon(E') = \int g(E', E) E dE$$

— average energy losses per a collision. Then in a relativistic case $\varepsilon(E) \ll E$ and the energy flux equation takes the following form

$$\frac{d}{dx} W(x) = -n \int \sigma(E) v(E) f(x, E) E dE. \quad (4)$$

2. Solution for the monoenergetic case without scattering

In a particular case of monoenergetic distribution electrons in each point of space have the same energy $\tilde{E}(x)$ and their distribution function $f(x, E) = N \cdot \delta\big(E - \tilde{E}(x)\big)$, respectively. N here determines normalization and can be found from a ratio of the energy flux W to the energy of an individual electron. In this case, the energy flux becomes proportional to electron's local energy $W(x) = N\tilde{E}\tilde{v}$, where $\tilde{v}$ is a velocity of the electron with the energy $\tilde{E}$. The flux equation takes the form that is similar to the Bouguer law for absorption of monochromatic light:

$$\frac{d}{dx} W(x) = -n\sigma(\tilde{E}) W(x) = -\frac{W(x)}{\lambda_{st}(\tilde{E})}. \quad (5)$$

When doing so, heating of the substance (per a unit volume) is calculated as $G = dW/dx$. The equation of the local beam energy has a similar form

$$\frac{d}{dx} \tilde{v}\tilde{E}(x) = -\frac{\tilde{v}\tilde{E}(x)}{\lambda_{\text{st}}(\tilde{E})}.$$

The magnitude λ_{st} characterizes the flight of the electron with this energy and can be experimentally measured from a ratio of an incoming energy flux to its losses in the substance („stopping power"). In the following we use approximation formulas presented in paper [29] for this quantity:

$$\lambda_{st} \cong 1.67 \frac{A(\gamma_b - 1)^2}{Z\rho_{gcc}\gamma_b f_{st}} \text{ [cm]},$$

$$f_{st} = 11.2 - 0.5 \ln\left(\frac{Z\rho_{gcc}}{A} \frac{\gamma_b}{(\gamma_b - 1)^2}\right), \quad (6)$$

where ε_b is energy of fast electrons, $\gamma_b = 1 + \varepsilon_b/(m_e c^2)$ is a gamma factor, $A = m_i/m_p$ is a mass number, m_i is the mass of the ion, m_p is the mass of the proton, ρ_{gcc} is the plasma density in [g/cm^3].

We will refer to the numerical solution of the equation (5) as an exact one. It can be solved with various methods. An explicit finite-difference method results in a scheme

$$\frac{W_{m+1} - W_m}{x_{m+1} - x_m} = -\frac{W_m}{\lambda_{st}(E_m)},$$

where the index m enumerates steps of a spatial mesh. This method losses stability when a mesh size is higher than the free path $x_{m+1} - x_m > \lambda_{st}(E_m)$, , hence, it can not be practically applied. The completely inexplicit scheme

$$\frac{W_{m+1} - W_m}{x_{m+1} - x_m} = -\frac{W_{m+1}}{\lambda_{st}(E_{m+1})}$$

requires conversion of the function $\lambda_{st}(E)$ for the solution and it can neither be applied in practice [30–32]. However, both the semi-explicit scheme

$$\frac{W_{m+1} - W_m}{x_{m+1} - x_m} = -\frac{W_{m+1}}{\lambda_{st}(E_m)},$$

as well as the finite-analytical method

$$\frac{d}{dx} W(x) = -\frac{W}{\lambda_{st}\big(E(x_m)\big)}$$

are absolutely stable and lead to close results [33].

3. Multi-group method

Let us discuss practical application of the multi-group method in the problem of heating the substance with the electron beam. The multi-group approach implies approximation of the distribution function over a certain discrete mesh along the electron energies $E_1, E_2, \ldots, E_N$ as a set of the groups $f_1, f_2, \ldots, f_N$ with fixed energy. At the same time, the total energy is varied by a transition of the electrons from one energy group into another. After discretization, the equation (3) and the magnitudes will take the following form:

$$v_i \frac{\partial}{\partial x} f_i = -\sigma_i n v_i f_i + \sigma_{i+1} n v_{i+1} f_{i+1},$$
$$f = n\delta_i^{i_0}, \quad (7)$$
$$W = \Sigma_i E_i v_i f_i = n E_{i_0} v_{i_0},$$

$$G = \sum_i (E_i - E_{i-1})\sigma_i n v_i f_i = (E_{i_0} - E_{i_0-1})\sigma_{i_0} n v_{i_0} f_{i_0},$$

where the index i is a number of the energy group, the index i_0 corresponds to the energy of the monoenergetic electron beam, σ_{i+1} is an effective collision cross-section that corresponds to energy losses $E_{i+1}-E_i$. Interrelation of σ_{i+1} with the experimentally measured magnitude λ_{st} can be found from considering energy losses of the monoenergetic beam. When the monoenergetic flow W with the energy E_0 propagates, the substance is heated with a power density W/λ_{st}. By equating $G = W/\lambda_{st}$ (and substituting i_0 with j for convenience), we obtain

$$\frac{E_j \cdot n v_j}{\lambda_{st}(E_j)} = (E_j - E_{j-1})\sigma_j n v_j f_j, \tag{8}$$

$$n\sigma_j = \frac{1}{\lambda_{st}(E_j)} \frac{E_j}{(E_j - E_{j-1})} = \frac{1}{\lambda_j}.$$

Thus, the equation of power of the electron flow in the beam will be like this:

$$\frac{dW_i}{dx} = -\frac{W_i}{\lambda_i} + \frac{E_i}{E_{i+1}} \cdot \frac{W_{i+1}}{\lambda_{i+1}}. \tag{9}$$

This system of equations is discretized similar to (5). Since the electrons transit only from the higher-energy groups into the lower-energy groups, the equations can be integrated by space subsequently, starting from an upper energy group. Let us designate $h_i = E_i/E_{i+1} \cdot W_{i+1}/\lambda_{i+1}$ — a volume energy flux from the energy group $(i+1)$ into the group i. For the upper group with an initial and, therefore, highest energy value, this magnitude is zero, for $i < N$ it is known from solving the equation in the group $(i+1)$. It can be found from energy balance:

$$h_{m,i} = \frac{E_{i-1}}{E_i} \cdot (W_{m-1,i} - W_{m,i} + h_{m,i+1} \cdot \Delta x),$$

where the first index designates a coordinate increment. By assuming that this flux is constant in the cell, we obtain semi-explicit and quasi-analytical discrete schemes:

$$\frac{W_{m+1,i} - W_{m,i}}{x_{m+1} - x_m} = -\frac{W_{m+1,i}}{\lambda_i} + h_{m,i},$$

$$W_{m+1,i} = \frac{W_{m,i} + (x_{m+1} - x_m)h_{m,i}}{1 + (x_{m+1} - x_m)/\lambda_i},$$

and

$$\frac{dW_i}{dx} = -\frac{W_i}{\lambda_i} + h_{m,i},$$

$$W_{m+1,i} = W_{m,i} e^{-(x_{m+1}-x_m)/\lambda_i} + \lambda_i h_{m,i}\left(1 - e^{-(x_{m+1}-x_m)/\lambda_i}\right).$$

The energy absorbed in the substance is energy not transferred into the lower group. It means that we can find distribution of the specific energy transferred per a unit volume in the i-the energy group as a difference between a value of the flux power before transition into the next group and a value after that. Hence, absorption in the substance is calculated as follows:

$$g_{m,i} = \left(1 - \frac{E_{i-1}}{E_i}\right) \cdot \frac{1}{\Delta x} (W_{m-1,i} - W_{m,i} + h_{m,i+1}\Delta x). \tag{10}$$

As soon as all the particles in the flow transit into the lower group with a new energy value, it is again calculated across an entire computational area for the next energy group unit the entire energy is absorbed in the substance. Therefore, the full energy being transferred to a unit volume of the substance is calculated as a sum of contributions from each group: $G_m = \Sigma_i g_{mi}$.

4. Convergence of the multi-group method to the exact solution

A problem of the multi-group method is its slow convergence to the exact solution for the monoenergetic beam. As an example, let us consider absorption of the monoenergetic beam with the initial energy $E_0 = 200\,\text{keV}$ in cold aluminum with the density of $2.678\,\text{g/cm}^3$ and the average ion charge $Z = 2.5$. The exact solution of the equation (5) for the monoenergetic beam without taking into account scattering, on a uniform mesh with the step of $1\,\mu\text{m}$ results in a typical distribution of absorbed power, which is similar to a Bragg peak for the ions. We note that taking into account electron scattering would result in widening of this peak.

This exact solution is compared with the solution of the multi-group equation (9) on the similar mesh with the various number of the groups in Fig. 2. As seen, in the multi-group method the peak is smeared and the less groups are used the wider the peak. It is also seen in the graph that convergence of the multi-group method takes place with a quite large number of the groups (about 1000) for the coordinate mesh size $\Delta x = 1\,\mu\text{m}$, wherein the found numerical solution substantially differs from the analytical one. Reduction of the mesh size and an increase of the number of the groups makes it possible to approach the exact solution.

5. Hybrid method

In the exact solution of the equation (5) all the particles in one point of space have the same energy, while in the multi-group approximation the particle flow is divided into groups by energies and the particles can have various values of the energy in one point. A lot of groups is required for convergence of the multi-group approach to the exact solution and obtaining in the calculations the Bragg peak to be observed when calculating the energy of absorption of electrons in matter in the approximation without scattering.

Let us construct a multi-group approach, in which unlike the usual multi-group approximation the value of the average energy inside the group is not fixed, but can be found

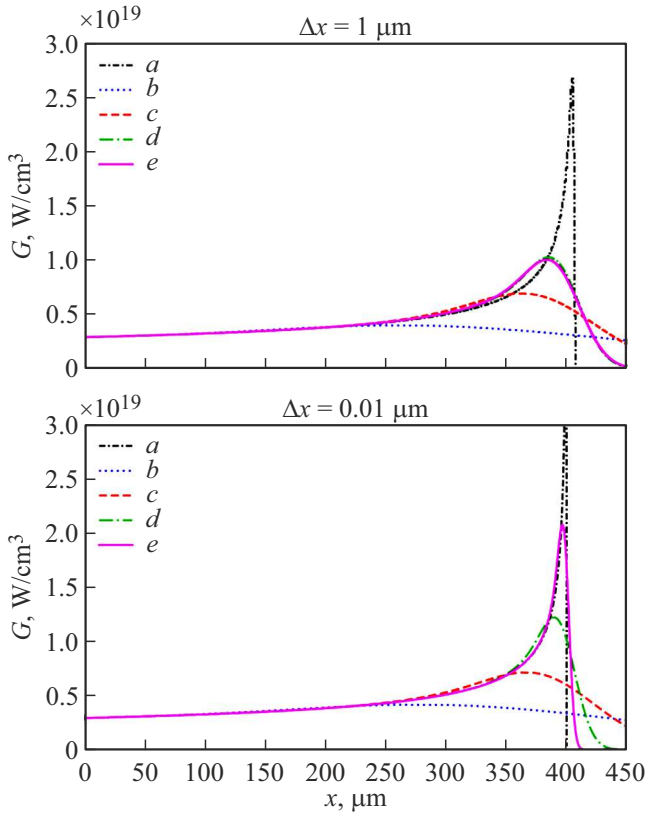

Figure 2. Distribution of absorbed energy in the exact (quasi-analytical) solution and for the multi-group approximation depending on the mesh size, the curves correspond to the numerical solutions: *a* — the exact solution, *b* — the multi-group method for 10 groups, *c* — 100 groups, *d* — 1000 groups, *e* — 10 000 groups.

from the solution of the equation. For this purpose, we set equations for the density of the particle flow $F_i = v_i f_i$ and for the density of the energy flux$W_i = \langle E_i \rangle v_i f_i$ in each energy group on the discrete space mesh. In case of no transition of the particles from one group into another, the dynamics of W is determined by the equation (5), while that of F is kept. Thus, the equation with transitional terms of the solution δW and δF is written as

$$W_{m+1,i} = W_{m,i} e^{(-(x_{m+1}-x_m))/\lambda_{st}} + \delta W_{m+1,i}, \qquad (11)$$

$$F_{m+1,i} = F_{m,i} + \delta F_{m+1,i}.$$

Here, the first index designates a group coordinates, so does the second one a group number; δW and δF determine a transition of a portion of the particles from the group $(i+1)$ into the group i. As long as the average energy in the group $\langle E_i \rangle = W_i/F_i$ is still above the lower boundary of the group E_i, the transitional terms δW and δF are zero. At the moment of the transition from group into group δW and δF are equal to current values of the particle flow and the energy flux: all the particles are thrown from this group into the lower one. The free path λ_{st} is determined exactly by $\langle E_i \rangle$, and it is not a fixed one unlike the multi-group approximation. Variation of the free path makes it possible to correctly describe presence of the peak.

Absorption of energy per a unit volume can be obtained from the obtained values of the flux power for each group in each point of space:

$$g_{m,i} = \frac{1}{\Delta x} \cdot (W_{m-1,i} - W_{m,i}), \qquad (12)$$

$$G_m = \sum_i g_{m,i}.$$

We note that here formulas for calculation of energy absorption are similar to expressions for the exact solution, since in both the methods the beam electron energy continuously varies.

If in the monoenergetic case the distribution function is described by one zero-width peak, and in the multi-group method it is described by a piecewise-constant function with fixed intervals, then in this approach it is a sum of a certain number of delta functions.

$$f = \sum_i N_i \cdot \delta\big(E - \langle E_i \rangle\big) = \sum_i \frac{F_i}{v_i} \cdot \delta\left(E - \frac{W_i}{F_i}\right).$$

It is obvious that on one group this method is completely similar to the exact solution for the monoenergetic spectrum. Presence of many groups makes it possible to describe a situation when one point of space includes electrons of different energies. This situation may happen, for example, if the monoenergetic beam reflects from boundaries of the target substance, when an incident beam and a doubly reflected beam propagate along one direction, but with different energies. The equation (5) can be used in this case, but instead of the x coordinate it shall include consideration of a coordinate along the ray, which is different for the incident beam and the reflected beam in the same point of space. In case of the two-dimensional problem, it necessitates calculation of electron trajectories or ray tracing.

The proposed multi-group method with continuous variation of the energy inside the group is trivially generalized to the multi-dimensional case, while in case of a foreign monoenergetic source it makes it possible to find the exact solution over a number of the groups, which is quite small as compared to the classic multi-group approach.

Computationally, when solving the one-dimensional problem, the method (11) is inferior in the speed to the quasi-analytical solution of the equation (5) and can be compared to the multi-group method (10) on the same number of the groups. At the same time, in case of presence of reflection the equation (5) can not be applied explicitly and convergence of the method (10) is attained on thousands of groups. The method (11) can be applied if the number of the groups is at least equal to a number of reflections of the electron beam from the target boundaries, which is below ten at the considered parameters for the target of the thickness $\sim 100\,\mu$m. Thus, for the problems with a small number of reflections of the beam from the target

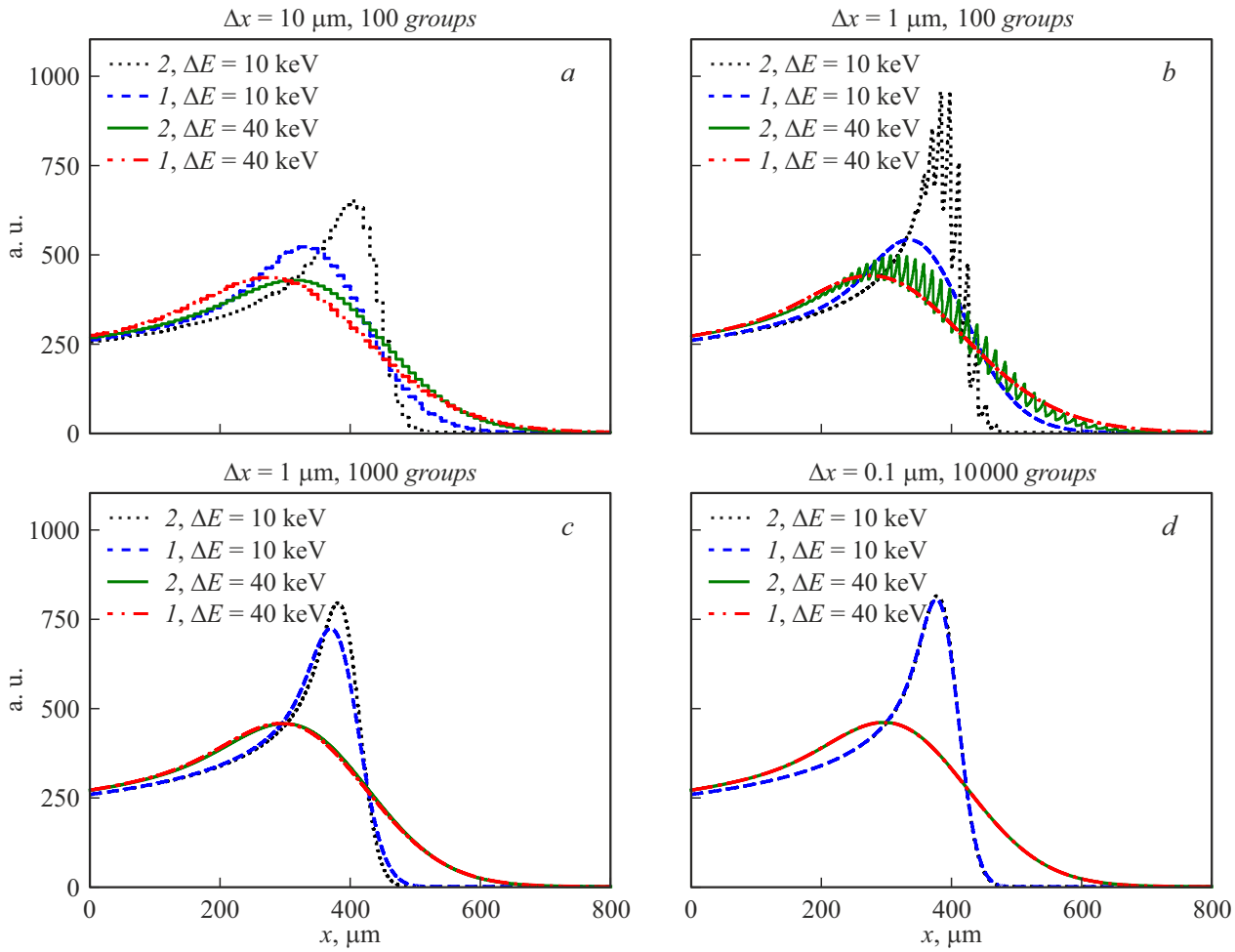

Figure 3. Distribution of absorbed power for the hybrid method and the multi-group method depending on the number of the groups and the mesh size for two options of initial energy distribution; the curves with the designation (*1*) correspond to the multi-group method (the number of the groups is shown in the graphs), the curve designation (*2*) corresponds to the hybrid method.

boundaries, the method (11) turns out to be essentially faster than the method (10). In case of the targets with the thickness $\sim 1\,\mu$m it is heated almost homogeneously and it is unreasonable to use the method (11).

6. Comparison of the multi-group approach and the hybrid approach in case of non-monoenergetic distribution

Now we consider not the monoenergetic spectrum of the beam, but a case of Gaussian energy distribution of electrons, in which $W_0 \propto \exp\left(-(E-E_0)^2/dE^2\right)$, wherein $E_0 = 200\,\text{keV}$ and $dE = 10,\ 20,\ 40\,\text{keV}$. In numerical calculations, the initial distribution function is discretely described and it is a sum of delta functions. In the hybrid approach, in case of the monoenergetic spectrum to be given by one delta function, energy absorption is described by one Bragg peak. Correspondingly, for the distribution function that will be given as a sum of delta function, a sequence of the absorption peaks will be observed. A depth, at which the major part of energy is absorbed in case of the monoenergetic beam, depends on the free path of electrons with energy E_i, the parameter $\lambda_{st}(E_i)$. For several monoenergetic beams with the different initial energies, which simultaneously irradiate the target, the Bragg peak will be observed at the different depth depending on $\lambda_{st}(E_i)$, where $i \in [1, N]$, N is a number of beams with different energies. If λ_{st} for the adjacent values in the energy mesh differ by more than the coordinate mesh size, then the Bragg peaks are separately observed, which does not correspond to physical description of the phenomenon in case of a continuous energy spread in the initial beam. Hence, the condition of convergence of this method: $\Delta x > |\lambda_{st}(E_i) - \lambda_{st}(E_{i+1})|$, where Δx is a mesh size and $\lambda_{st}(E_i)$ is a free path of the electron with energy E_i. In the multi-group approach, this numerical defect is not observed due to smearing of the absorption peaks and convergence of the method will not be disrupted if the above condition is not fulfilled. It is clear from Fig. 3, *d* that when the number of the groups is increased and the

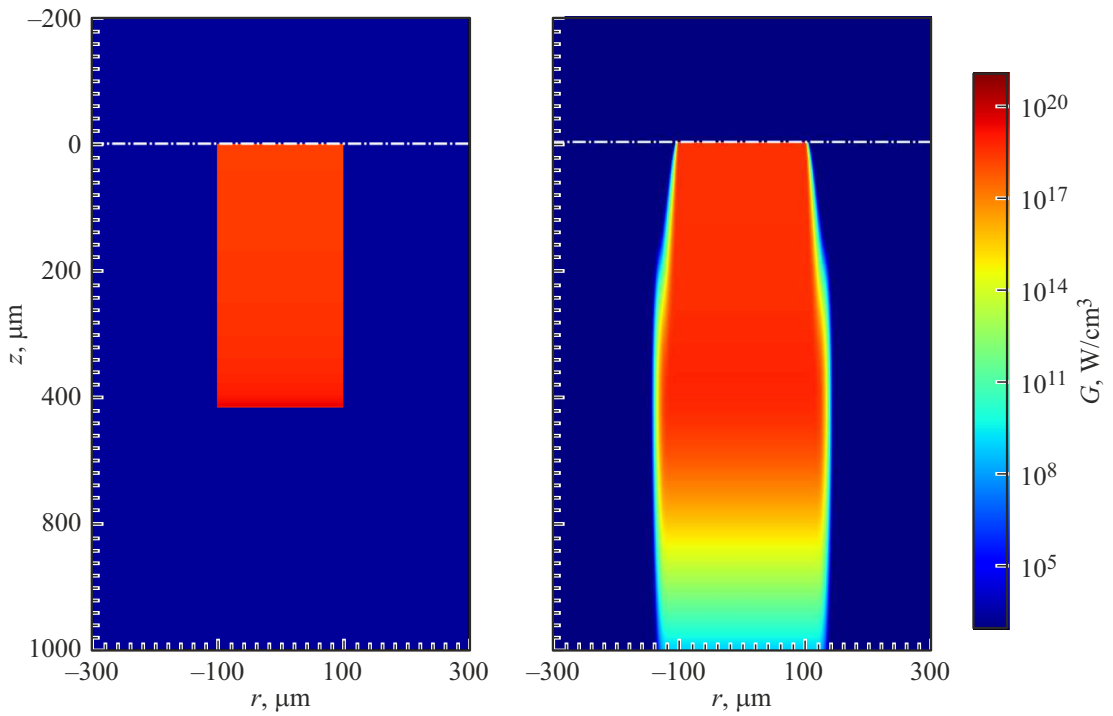

Figure 4. Absorbed power calculated by the hybrid method (to the left) and in the multi-group approximation (to the right) at the initial moment of time in logarithmic scale.

condition of convergence is fulfilled, the numerical defect disappears and the solutions obtained by means of the hybrid method and the multi-group method converge.

When the distribution is closer to the monoenergetic one and the condition of convergence for the mesh size is satisfied, it is clear (Fig. 3, *c*) that with the increasing number of the groups the hybrid method converges faster than the multi-group one, i.e. the closer the distribution to the monoenergetic one, the better the hybrid method converges. The multi-group method requires a finer mesh and a higher number of the groups for convergence. But when there is no fulfillment of the condition for the mesh size and a step between λ_{st}, the hybrid method no longer works correctly and a typical ridge is observed, where each energy absorption peak corresponds to a delta-function input beam with energy that corresponds to one of the values of the group-divided spectrum. This numerical defect is critical in calculations of hydrodynamics.

Using the hybrid method is more preferable than use of the multi-group method, when the initial spectrum is close to the monoenergetic one. It works better than the multi-group one at $\Delta E < 0.1E$, when divergence of the initial beam is about 10 %. It is important that with high resolution of the space mesh a larger number of the energy groups is required. Otherwise, the method diverges and description of energy input becomes fundamentally non-physical. No such problem exists in the multi-group method, with the increasing space mesh the solution ceases to converge to the exact one and the absorption peak turns out to be smeared, thereby resulting in underestimation of a shock-wave amplitude.

7. Influence of a calculation method on target gas dynamics

Dynamics of irradiation of the solid-state aluminum target with the electron beam has been numerically modelled in RZ-geometry in the hybrid approximation and in the multi-group energy approximation. The 3DLINE software with radiation gas dynamics [34] had a numerical module of taking into account electron beam heat transfer embedded and it was tested based on the multi-group method and the hybrid method. Thermodynamic parameters were calculated as a function of the density and the temperature according to a semi-empirical FEOS package [35,36] based on the Thomas–Fermi model. Thermal radiation transfer coefficients were calculated in a collisional-radiational model by the THERMOS code [37]. The monoenergetic parallel electron beam was hitting the target at the right angle, the electron energy was 200 keV, flux intensity was $2 \cdot 10^{17}$ W/cm^2 and a beam radius $R = 100\,\mu$m. Simulation was done for a semi-infinite aluminum target with the room temperature and the density of 2.678 g/cm^3. In simulation, electron beam irradiation lasted for the entire calculation time.

Distributions of absorbed power at the initial moment of time, which are obtained in these two approximations, are shown in Fig. 4 (in volume the electron beam hits the target

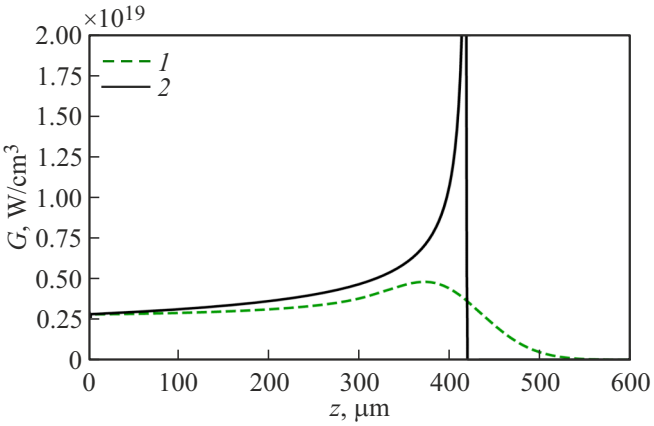

Figure 5. Absorbed power at the initial moment of time depending on the distance to the target surface; *1* — the solution by the multi-group method (100 groups), *2* — the solution by the hybrid method (the exact solution).

from above, a target surface is dash-dotted) and Fig. 5 (as a function of a distance to the target surface). Hereinafter, zero of the z axis is matched with a position of the target surface at the initial moment of time, so are positive values of the z axis with the depth.

A difference between the methods is manifested in two aspects: the already discussed widening and smearing of the absorption peak in the multi-group method (Fig. 5 and 2) a new, essentially two-dimensional effect: numerical diffusion in a direction perpendicular to beam propagation for the multi-group method. This effect results in widening of the beam and reduction of average intensity in it, hence even before the absorption peak Fig. 6 exhibits differences in absorbed power.

Influence of these two numerical effects on dynamics of the target substance can be demonstrated by comparing two-dimensional density distributions at the various moments of time, which are shown in Fig. 6. Dynamics of dispersion of matter into vacuum is described identically in both the approximations. It is an expected effect, since essential differences between the methods are observed near the absorption peak and for the time considered their influence has no enough time to affect dynamics of matter near the surface. It is also true for the shock wave propagating in a beam-perpendicular direction: if considering a cross section far away from the absorption peak, then the values of the shock-wave amplitude, which are obtained in these two calculations, will turn out to be close.

Basic differences are observed near the absorption peak (Fig. 7). Due to almost complete absence of „a tail“ after the peak, a temperature gradient (hence, a pressure one, too) in the hybrid method is entirely caused by processes of thermal conductivity (both electron one as well as radiative one), whereas for the multi-group method, there is a typical scale caused by an absorption profile. It results in multiply different amplitudes of a shock wave propagating from the absorption peak. In the hybrid method with the narrow peak of energy absorption a substance compression degree reaches 10, whereas in the multi-group method it is below 5% due to widening of an energy input region. At the same time, the total input energy is the same in both the cases.

Influence of this „explosion“ in the target bulk also affects the shock wave in a direction perpendicular to propagation of the electron beam. Respective distributions of the density at the depth of 100 μm (near the position of the absorption peak for the hot substance) at the various moments of time are shown in Fig. 8. The difference between the methods in this respect is weaker, since in the perpendicular direction a sharp gradient also exists in the multi-group method, albeit it is blurred by numerical diffusion. Nevertheless, when using the multi-group method, the substance compression ratio is reduced from 4.5 to 2.6.

Conclusion

The study has considered the solution of the problem of heating the dense target with the monoenergetic electron beam in the multi-group energy approximation and the improved (hybrid) energy approximation. Application of the classic multi-group method requires not only a large number of the groups for convergence to the exact solution, but a detailed space mesh — noticeable divergences start in a region where the electron free path becomes comparable to the mesh size. Thus, an unavoidable effect is widening and smearing of the absorption peak, thereby resulting in noticeable differences in calculations of target dynamics: the temperature gradient along the beam propagation direction, which determines intensity of the shock wave, depends on numerical parameters of the calculation (the number of the groups and the mesh size).

The modification of the multi-group method („the hybrid method“), which is based on simultaneous tracking of both the number of particles as well as the energy flux in each group, results in convergence to the exact solution over the small number of groups. This method makes it possible to calculate beam energy absorption in the problem with boundary conditions of reflection without tracing separate electrons. A disadvantage of the method is a limitation on the minimum number of groups to be taken into account: it should be not less than the maximum number of electron reflections from the target boundaries. Its advantage is that it can be simply generalized for the case of the multi-dimensional problem and it is possible to take into account scattering without using the Monte Carlo method.

Based on the designed method, we have modified the 3DLINE RGD-code and calculated dynamics of the infinitely-thick aluminum target under impact of the electron beam with energy of 200 keV with intensity of $2 \cdot 10^{17}$ W/cm^2. The calculation was compared with the results obtained in the multi-group approximation on 100 energy groups. The energy absorption difference in the

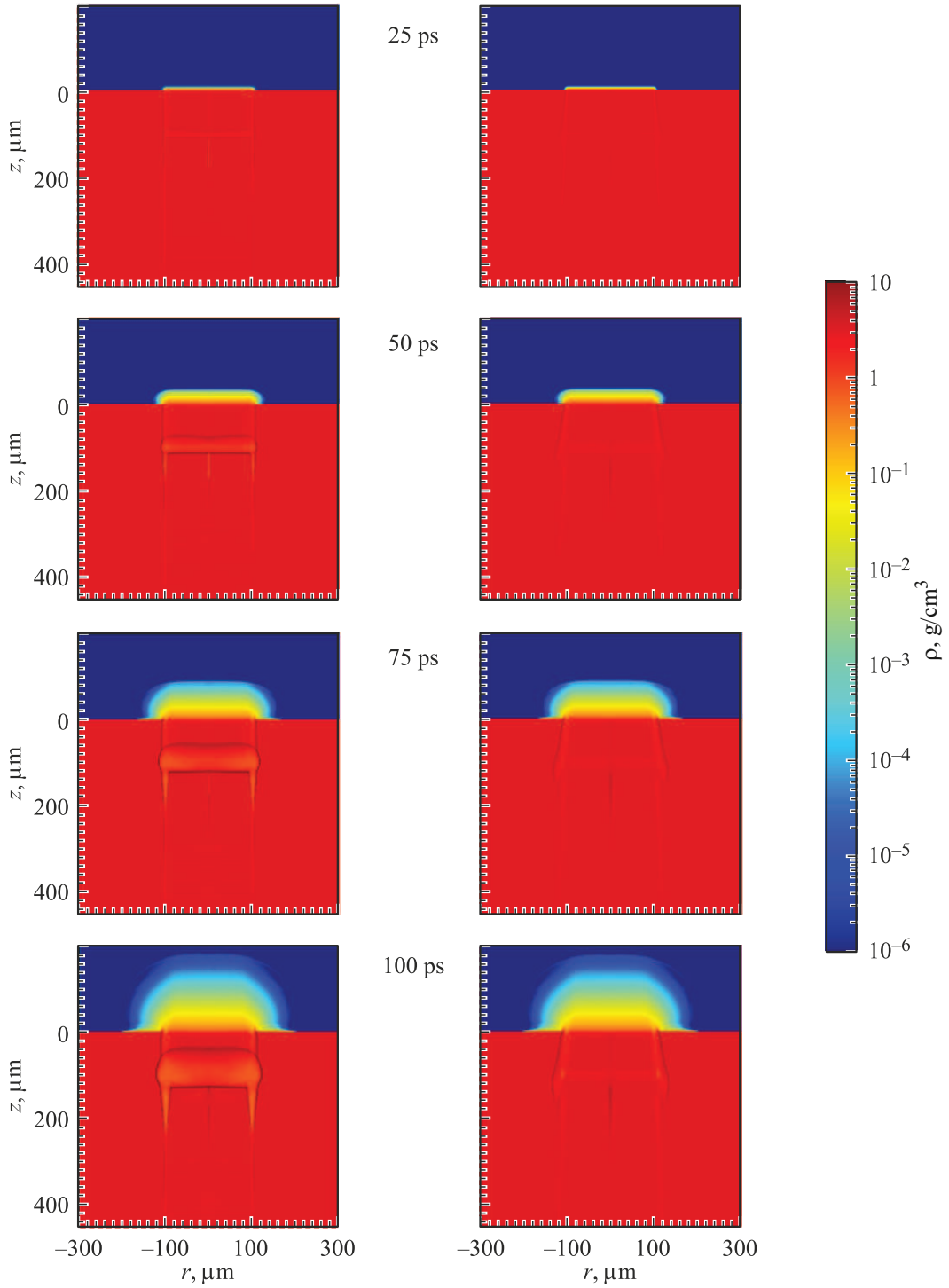

Figure 6. Density profiles calculated by the hybrid method (to the left) and in the multi-group approximation (to the right) at the various moments of time (25, 50, 75, 100 ps) in logarithmic scale.

two methods results in significant differences of heating and dynamics of propagation of shock waves in matter. There is a multiple difference in amplitudes for the shock wave propagating along the beam, whereas for the wave in the perpendicular direction the differences are not so essential.

Thus, the hybrid method turns out to be more effective in the problems that require considering matter irradiation with the monoenergetic or close-to-monoenergetic electron beam. The proposed approach makes it possible to reach high accuracy of calculations with significantly lower computational costs, which is important for simulating complex physical processes. The observed significant differences in dynamics of shock waves, especially along the beam propagation direction, demonstrate critical influence

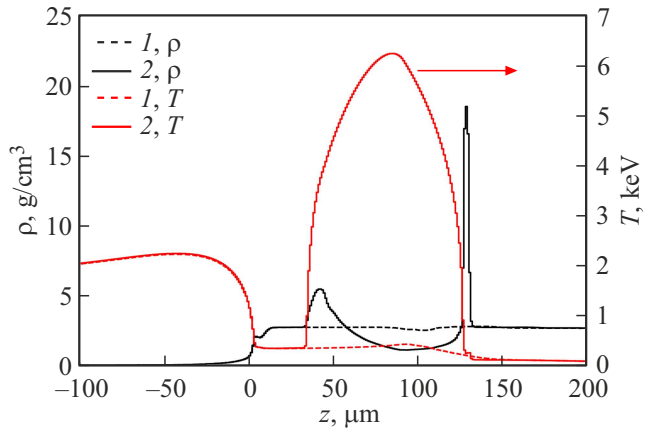

Figure 7. Temperature and the density along the z axis, which are calculated by the hybrid method (the solid lines) and in the multi-group approximation (dashed) in 100 ps after start of irradiation.

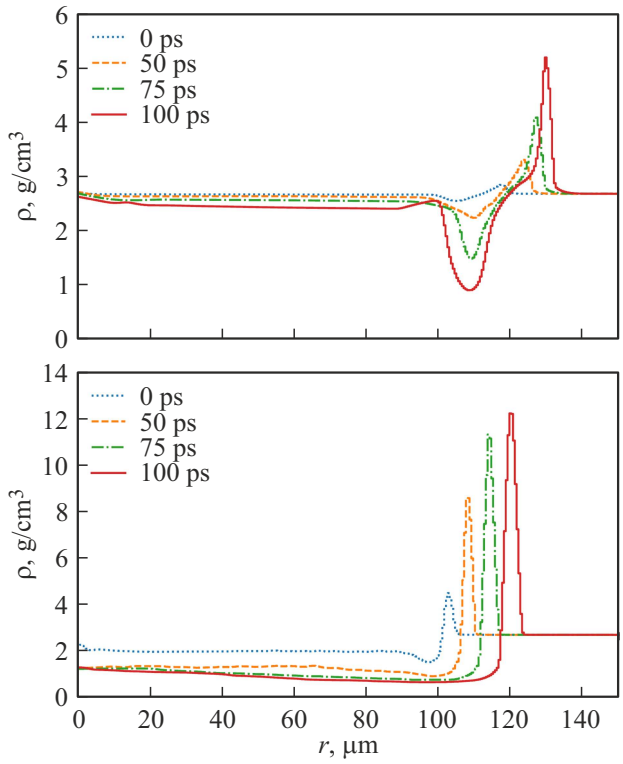

Figure 8. Distributions of the density in the cross section at the depth of 100 μm, which are obtained by the hybrid method (above) and in the multi-group approximation (below) at the various moments of time.

of accuracy of energy absorption on the final result of simulation.

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Conflict of interest

The authors declare that they have no conflict of interest.

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