УДК: 004.942:519.6

Methods of calculating the partial derivatives of the electron radiation dose measured with dosimetric wedge

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In the work, the numerical methods of determining the standard characteristics of the electron radiation depth-dose distribution by processing the measurement results are compared with the empirical formulas linking the same characteristics with the electrons energy. The comparison results allow authors to estimate the accuracy of methods used in radiation technologies to determine the characteristics of electron radiation energy.

Key words: *electron radiation, depth-dose distribution, numerical methods, semi-empirical model, empirical formulas.*

У роботі проведено порівняння чисельних методів обробки результатів вимірювань для визначення стандартних характеристик глибинних розподілів дози електронного випромінювання і емпіричних формул, що зв'язують ці характеристики з енергією електронів. Результати порівняння дозволяють оцінювати точність визначення характеристик енергії електронного випромінювання, методами, які використовуються в радіаційних технологіях.

Ключові слова: *випромінювання електронів, розподіл дози по глибіні , чисельні методи, напів-імперична модель, імперичні формули.*

В работе проведено сравнение численных методов обработки результатов измерений для определения стандартных характеристик глубинных распределений дозы электронного излучения и эмпирических формул, связывающих эти характеристики с энергией электронов. Результаты сравнения позволяют оценивать точность определения характеристик энергии электронного излучения методами, которые используются в радиационных технологиях.

Ключевые слова: *излучение электронов, распределение дозы по глубине, численные методы, полу-импирическая модель, импирические формулы.*

Introduction

The necessity to improve existing and to develop new methods for determination and auditing radiation process parameters is associated with expansion of application of radiation technologies. The accuracy and informativeness of methods for determining parameters can be significantly increased due to development of software for processing the results of measurements, performed on existing equipment.

It should be noted, that improvement of accuracy and informativeness of computational methods is not possible without use of physical regularities in the computing algorithms. Therefore, study of possibilities to use empirical regularities for development of improved algorithms for processing the measurement results is an actual task.

The energy of electrons is one of actual parameters of electron beams radiation facility. In the standards [1,2], the formal procedures is discussed, which is intended for determining the most probable energy E_p of electron beam on basis of an

empirical relationship $E_p(R_p)$ and calculation of practical range R_p of electrons according to the relations:

$$R_p = x_p - \frac{D(x_p) - D_{rad}}{D'(x_p)} \qquad x_p = \arg\max_{x\in[Rm,Ro]}(-D'(x)) \tag{1}$$

Here $D(x)$ and $D'(x)$ are dose distribution and derivative of dose with respect to depth, D_{rad} is the value of extrapolated dose of electron bremsstrahlung.

However, the results of measurements of electron depth-dose distribution by dosimetric wedge or stack, which are used in the radiation technological centers, are a set of discrete data. Therefore, the formal procedures for determination of energy of electrons require solutions of incorrect mathematical task – numerical differentiation of dose distribution of electrons.

Comparison of methods of electron radiation dose numerical differentiation, which use various approximations of discrete data sets, was reported in [3]. In this work, the values of both the first and the second derivatives were calculated by polynomial approximation methods and the fit of semi-empirical model to the results of numerical experiments.

The results of numerical experiments, which are used in this work, were obtained by RT-Office software [4] with a very small relative statistical error (<0.01%). The results show that methods of fitting the semi-empirical models or polynomial approximation of experimental data allow with sufficient accuracy to calculate values of the first derivative of dose distribution with respect to depth. However, the same computational methods are only suitable for estimates when it goes about determining values of the second derivative of depth-dose distribution.

It should be noted, that electron energy control procedure in the process of radiation treatment of objects is associated with the need to keep the energy of electrons in a certain range. This range of electron energy values in a beam is determined by conditions imposed on dose value distributed in the irradiated object.

For example, for radiation sterilization processes, such conditions include:

- the minimum dose value in the irradiated volume Ω should be greater than some certain predetermined value D_{st} (sterilization dose) required to perform radiation sterilization process

$$\min_{x\in\Omega}(D_M(x,E)) \geq D_{st} \tag{2}$$

- dose uniformity level in the irradiated volume Ω, which is defined as ratio of maximum to minimum dose in this volume, should not exceed a predetermined value DUR required for performing the radiation sterilization

$$\frac{\max_{x\in\Omega}(D_M(x,E))}{\min_{x\in\Omega}(D_M(x,E))} \leq DUR \tag{3}$$

Here $D_M(x,E)$ is the depth-dose distribution of electron radiation in material M resulted from electron irradiation with energy E.

The above conditions are used for determination of an electron beam energy boundaries allowed for irradiation process. At optimal planning of the irradiation process, the range of electron beam energy changes ΔE is determined by values $\Delta D(x_c)$ – uncertainty of dose measurements – in the critical spatial points x_c, which are the points of maximum and minimum of electron radiation dose.

Therefore, when planning radiation sterilization process, the permissible range of electron energies is defined as the actual parameters of radiation installations, and as characteristics of the objects to be sterilized. For small uncertainty of dose measurement results $\Delta D(x_c)$, the allowable energy range of electrons ΔE is determined by partial derivative of the doses $D_M(x,E)$ with respect to electron energy

$$\Delta E = \Delta D(x_c) \cdot \left(\frac{\partial D_M(x_c, E)}{\partial E} \right)^{-1}. \quad (4)$$

Therefore, an actual task is development of computational methods for determining partial derivatives of electron radiation dose with respect to electron energy, based on results of measurements performed with standard methods in industrial sterilization centers.

Formulation of the problem

Unlike the measured depth-dose distribution in the irradiated object that can be used for numerical differentiation of dose with respect to depth, the experimental data of dose dependence on energy of electrons are not available in industrial sterilization centers. In this regard, one of the key tasks of computational dosimetry, is development of computational methods for determining the partial derivatives of the dose distribution with respect to energy of electron radiation.

In this paper, the authors evaluate the possibility to use a semi-empirical model of electron energy absorption in a substance for calculation of the partial derivative of the dose distribution with respect to electron radiation energy.

The methods of processing depth-dose distribution measured with dosimetric wedge for determining the partial derivatives of electron radiation dose were considered.

Particular attention was paid to the method of determining the acceptable changes in electron beam energy, based on results of measurements performed by standard methods in industrial sterilization centers.

Calculation of partial derivatives of dose with respect to energy of electrons

To determine the partial derivative of electron radiation dose in a substance with respect to electron energy, the authors have simulated the depth-dose distributions resulted from the substance irradiation by monoenergetic electron beams of various energies. Transport of electrons in the matter was simulated on the base of RT-Office

software [4] by the Monte Carlo method implemented in a detailed physical model using.

The energy values of monoenergetic electron beams used for this purpose represented two different sets: (4.95, 5, 5.5) and (9.9, 10, 10.1) MeV. The simulated distributions of depth-dose $D_M(x,E)$ absorbed in various irradiated materials, such as polyethylene, carbon, water, teflon, wood, aluminum, have shown small relative statistical error (<0.03%).

In the parallel, the partial derivatives of electron radiation dose were calculated by the standard computational methods for electron energies E = 5 and 10 MeV.

It was shown that, if the simulation results have small relative statistical error, the partial derivative $\partial D_M(x,E)/\partial E$ can be calculated on the base of modeled depth-dose distributions using the standard computational methods like Monte Carlo method.

To illustrate this conclusion, Figure 1 shows the partial derivatives of electron radiation dose as depth function in polyethylene at electron energies 5 MeV (triangles), and 10 MeV (circles).

The values of partial derivatives of doses with respect to electron energy E – $\partial D_M(x,E)/\partial E$ – as a function of depth x of absorption energy of the electron radiation. To illustrate results, in Fig. 1 it is shown the derivatives of electron radiation dose as function depth in polyethylene for 5 and 10 MeV electron energies.

Resulted from electron radiation of the studied substances and electrons energies, were calculated using a computer implementation [5] semi-empirical model.

Calculations were performed in a semi-empirical model (solid lines) as well as by numerical differentiation of discrete data obtained by the Monte Carlo method (points). The vertical dotted lines mark the depths corresponding to the peaks of electron radiation dose derivatives. As can be seen in Fig. 1, at these depths, the dose values are close to the half value of the maximum dose in target.

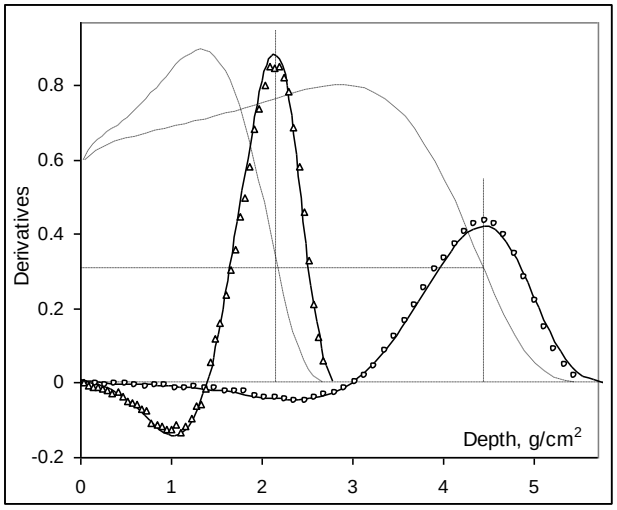

Fig.1. Partial derivatives of electron radiation dose as depth function in polyethylene target, for 5 MeV electron energies (triangles) and 10 MeV (circles).

Points represent calculations based on numerical differentiation of data obtained by the Monte Carlo method. Solid curves correspond to calculation based on semi-empirical model of absorption energy of electron radiation. Dashed curves show depth-dose distributions of electron radiation for the electron energies of 5 and 10 MeV.

Comparison of results calculated on basis of numerical differentiation of discrete data, obtained by the Monte Carlo method [4] having small statistical errors as well as on basis of computer realization [5] of semi-empirical models of electron radiation dose shows their good agreement. Thus, it was demonstrated that it is possible to calculate the partial derivative of electron radiation doses with respect to electron energy using a semi-empirical model of energy of electrons absorbed in the target.

Calibration symmetry of depth distribution for electron radiation dose

The conclusions presented in the paper [3] and in the previous section of this paper show the possibility to use a semi-empirical model of absorption of electron energy in the target for calculation not only the depth-dose distribution of electron radiation, but also the partial derivatives of dose with respect to depth target and the electrons energy.

However, these conclusions are based on those cases, when well established correlation between parameters of the semi-empirical model and parameters of the computational experiments are obtained with small statistical errors.

In practice of dosimetric control, the measurement results can have significant random errors and uncertainty in determination of model parameters of the process under control can have greater values. That is why it is interesting to consider the empirical regularities that appear in the distribution of electron radiation dose as a function of target depth and the electron energy in beam.

One of empirical regularities is the so-called calibration symmetry (scale symmetry) of the depth-dose of mono-energetic electron radiation distribution.

The substance of calibration symmetry is that selection of special units for depth in dependence on the electron energy results in good coincidence of dose values as depth function over the decrease (reduction) interval of electron radiation dose distribution.

Fig. 2 shows a set of depth-dose distributions in the polyethylene for mono-energetic electron fluxes with energy E = 3, 5, 8, 10 and 12 MeV. For each value E of energy of electrons, the value of target depth X is defined in terms of $R_{ex}(E)$ - extrapolated range of the electrons in the target material [1]. Depth-dose distributions for different electron energies were calculated at fixed values of integral flow of electrons at the target surface (constant fluency of electrons).

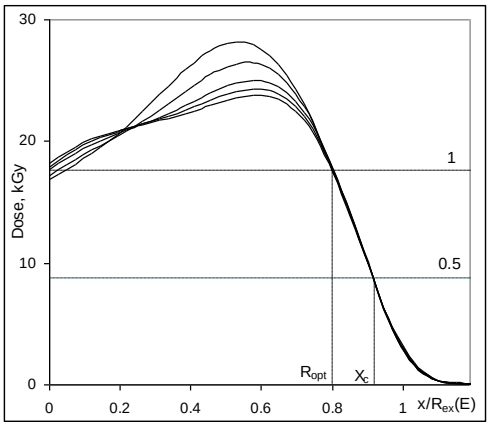

Fig. 2. Depth-dose distribution of the electron radiation dose in polyethylene for monoenergetic electron beams with energy E = 3, 5, 8, 10, 12 MeV.

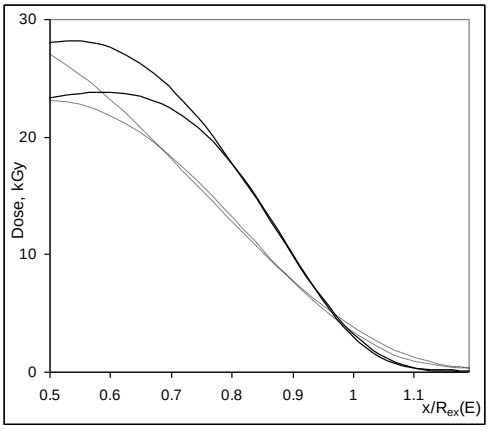

Fig. 3. Depth-dose distribution of the electron radiation dose in polyethylene (solid curves) and aluminum (dashed curves) for monoenergetic electron beams with energy E = 3 and 12 MeV

As can be seen from the Fig. 2, there is good agreement between the depth-dose distribution values over the depth range where the dose decreases moving away from the target surface (the horizontal dotted -1) up to $R_{ex}(E)$. A similar form have the dose distributions for substances (polyethylene, carbon, water, teflon, wood, aluminum), at irradiating by monoenergetic electrons with energies ranging from 3 MeV up to 12 MeV.

Fig. 3 presented dose distributions in polyethylene (solid curves) and aluminum (dashed lines) at the energy levels of 3MeV and 12MeV. Figure 3 shows, that the calibration symmetry is observed for various target substances and with increasing the effective atomic number of the target material dose rate of slope decreases.

As can be seen from Figs. 2 and 3, the area of depths, in which there is observed the calibration symmetry, has a relatively small size from 0.8 to 1.0. However, in this area the depth and size of dose is reduced greatly, and this area is of primary interest in the planning phase of radiation sterilization in determining the thickness of the object undergoing treatment. Exactly in this area is located critical point x_c of dose electron radiation, in which should be carried out calculations of allowed area the electrons energy ΔE, in accordance with (4).

At Figure 2 for processing objects made of polyethylene, it is marked the optimum thickness of the object R_{opt} (the point at which the magnitude of the dose is equal to the dose on the front target boundary) at one-sided irradiation and depth of critical point location X_c (the point at which the magnitude of the dose equal to half the dose values on the front boundary of the target) at two-sided irradiation facility.

Let us suppose that we have the following identities:

$$D_M(x,E) \equiv D_M^*(z(E)), \qquad z(E) \equiv x / R_{ex}(E), \tag{5}$$

for the area depth x in which there is a calibration symmetry of the dose distribution.

Under this assumption, the partial derivatives of the dose distribution with respect to energy and depth, may be represented as:

$$\frac{\partial D_M(x,E)}{\partial E} = \frac{-x}{R_{ex}^2(E)} \cdot \frac{dD_M^*(z)}{dz} \cdot \frac{dR_{ex}(E)}{dE} \tag{6}$$

$$\frac{\partial D_M(x,E)}{\partial x} = \frac{1}{R_{ex}(E)} \cdot \frac{dD_M^*(z)}{dz} \tag{7}$$

From equations (6) and (7) follow the relationships between the partial derivatives

$$\frac{\partial D_M(x,E)}{\partial E} = -z(x,E) \cdot \frac{dR_{ex}(E)}{dE} \cdot \frac{\partial D_M(x,E)}{\partial x} \tag{8}$$

Equation (8) provides a great practical interest, since it allows to calculate the partial derivative of dose with respect to energy electrons $\frac{\partial D_M(x,E)}{\partial E}$ with use of partial derivative of dose $\frac{\partial D_M(x,E)}{\partial x}$, which can be determined based on the measurement results performed by a dosimetry wedge [3].

For realization of relation (8) in the method of calculating the partial derivative of dose with respect to the electron energy, it should be determine the value of derivative extrapolated range of electrons with respect to the electron energy. The value of extrapolated range the electrons $R_{ex}(E)$ is well known [1] and there are empirical relationships to calculate the value of this quantity in various materials and for different electron energies.

It were calculated the values of extrapolated ranges of electrons $R_{ex}(E)$ in the following materials - polyethylene, carbon, wood, water, teflon, aluminum for electrons energies in the range from 2 up to 12 MeV, using the block "Analytics" in the software RT-Office [4]. Approximation of the extrapolated range with the use of linear functions on the electron energy has been implemented. The coefficients of linear functions $R_{ex}(E) = A_M \cdot E + B_M$ for various materials are shown in the Table 1.

Table 1. The coefficients of linear approximation for dependence extrapolated range of electron (in g/cm^2) on the electron energy (in MeV).

	Polyethylene	**Carbon**	**Wood**	**Water**	**Teflon**	**Aluminum**
A_M	**0.5046**	**0.5626**	**0.5348**	**0.5086**	**0.5773**	**0.5431**
B_M	**- 0.0993**	**- 0.1568**	**- 0.1414**	**- 0.1379**	**- 0.185**	**- 0.205**

Using the relation (8) and the assumption of a linear dependence of the extrapolated range on the electrons energy, we obtain the equation

$$\frac{\partial D_M(x,E)}{\partial E} = -\frac{x \cdot A_M}{A_M \cdot E + B_M} \cdot \frac{\partial D_M(x,E)}{\partial x} \qquad (9)$$

As follows from the data given in the Table 1 for the electron energy from 5 to 10 MeV the contribution coefficient B_M to the value of the extrapolated range of electrons is not great, for all above materials.

Numerical verification of the relationship between the partial derivatives (9), was performed on the basis of data on the depth distribution of electron radiation dose, obtained using the Monte Carlo method and the semi-empirical model of the absorption energy of electrons.

Testing results of various calculation methods of derivatives doses with respect to electron energy for the polyethylene target irradiated by electrons with an energy of 5MeV and 10MeV, are shown in Figs.4 and 5, respectively.

Points - the derivatives of the electron energy dose calculated based on dose distributions which were obtained by the Monte Carlo method.

Unfilled circles - the results of numerical differentiation of a set of discrete data with respect to the electron energy. These results are consistent with those shown in Fig. 1.

Filled circles – the results based on numerical differentiation of dose distribution with respect to depth and the use of the relationship between the partial derivatives(9).

Solid curves - derivative of doses with respect to electron energy, derived with use semi-empirical model of electron dose.

These results were obtained by a numerical differentiation doses with respect to energy (the same as given in Fig. 1) and using the relation (9) based on the numerical differentiation of dose with respect to depth.

From the Figures it is clear, that significant differences in the results obtained by different methods are observed only in the field of violation of calibration symmetry dose distributions, that is, according to the data presented in Fig.2, to the depths $x < 0.6 \cdot R_{ex}(E)$. Comparison dependencies shown in Fig.4 with similar to that in Fig.5 shows that in area depths, where there is a calibration symmetry, the values of derivatives is inversely proportional to electron energy.

Using the expression (6) and the assumption of a linear dependence of extrapolated range on electron energy, the partial derivative of dose with respect to energy present in the form of:

$$\frac{\partial D_M(x_c,E)}{\partial E} = \frac{-z_c \cdot A_M}{A_M \cdot E + B_M} \cdot \frac{dD_M^*(z_c)}{dz}, \qquad z_c = x_c / R_{ex}(E). \quad (10)$$

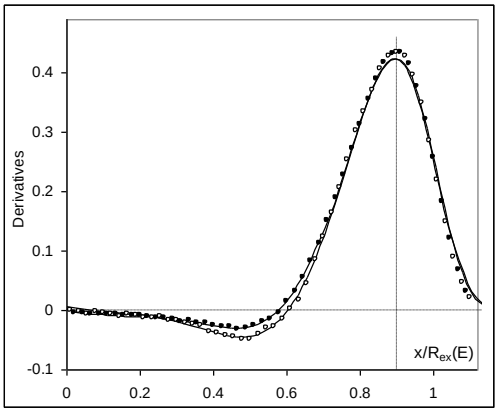

Fig. 4. Partial derivatives of electron radiation dose with respect to the electron energy, obtained by different computational methods for polyethylene target irradiated with 10 MeV electrons

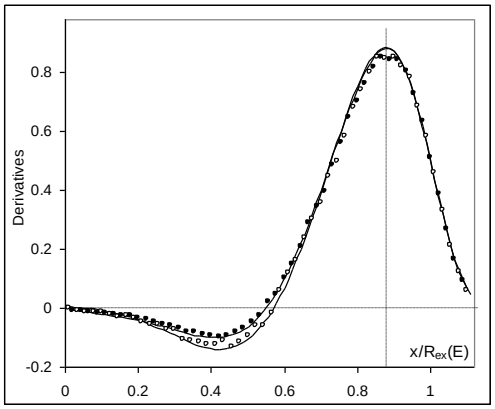

Fig. 5. The partial derivatives of electron radiation dose with respect to the electron energy, obtained by different computational methods for polyethylene target irradiated with 5 MeV electrons

It should be note that the value z_c of slightly varies with the electron energy and for electron energy range from 5 to 10 MeV into force $B_M << A_M \cdot E$ (see. Table 1), it can be assert, that the value $\eta_M(x_c, E)$ weakly depends on electrons energy

$$\eta_M(x_c, E) = E \cdot \frac{\partial D_M(x_c, E)}{\partial E}.$$

Whence it follows that the allowable relative change in the electron energy $\frac{\Delta E}{E}$ at the critical points z_c (see (4)) is determined by the target substance and is weakly dependent on electrons energy.

$$\frac{\Delta E}{E} = \frac{\Delta D(x_c)}{\eta_M(x_c, E)} \tag{11}$$

This conclusion was confirmed by a series of calculations.

Conclusions

By the numerical experiments, the method was demonstrated for calculating the partial derivative of the dose with respect to energy of electron radiation. The method is based on a semi-empirical model of absorption of electron energy in substance. This allows for solving optimization problems to obtain the necessary data within framework of semi-empirical models instead of simulation with Monte Carlo method, which works when statistical errors are small that significantly reduces the laboriousness for planning and monitoring of radiation-technological process.

On the basis of empirical regularities for depth-dose distributions of electron radiation, the relations between the partial derivative of the dose with respect to electron energy and the partial derivative of the dose with respect to depth were obtained. It was performed Verification of these relations was made on the basis of data on depth-dose distributions of electron radiation obtained by the Monte Carlo method and by semi-empirical model of electron energy absorption.

The verification results have allowed us to offer the method for calculating the derivatives of dose with respect to electron energy and evaluating the region of tolerance of electron energy changes during irradiation using the results of measurements performed by standard methods in industrial sterilization centers.

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Надійшла – 15.06.2016.