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Spatial Distributions of the Dose Created Phantom Pencil Beam of Mono-Energy and Bremsstrahlung Photons in a Water with Energies from 0.25 to 20 MeV

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ABSTRACT

Purpose: Critical analysis of existing and obtaining more accurate data on the spatial dose distributions created in the water phantom by pencil beams (PB) of monoenergetic and bremsstrahlung photons with energies from 0.25 to 20.0 MeV, and approximation of these distributions for the purpose of calculating doses in radiation therapy.

Material and Methods: Using the Monte Carlo method, the EGSnrc program and the MATLAB mathematical package, these distributions were calculated for monoenergetic photons in the energy range from 0.25 to 19.75 MeV in increments of 0.5 MeV, for bremsstrahlung photons with a maximum energy of 4.0, 6.0, 10.0, 15.0, 18.0 MeV and for the gamma-radiation spectrum of the therapeutic apparatus ROCUS. The calculation results are converted into the so-called dose kernel of photon pencil beam. The obtained dose kernel values are compared with previously published data and the observed discrepancies are discussed. Depths in water were studied from 1.0 to 40 cm in increments of 0.5 cm and along the radius from 0.02 to 46.0 cm with an uneven grid. For bremsstrahlung and photons with the spectrum of the ROCUS apparatus, the possibility of approximating dose kernel values using approximation formulas convenient for calculating doses in radiation therapy has been investigated.

Results: On the basis of the results obtained, a new version of the library of dose kernels of a pencil photon beam for water was created, which differs from previous versions by the use for calculating a better description and modeling of the physical processes of the interaction of photons and charged particles with matter, more adequate data on the interaction cross sections and significantly lower values of statistical uncertainties of the results. For bremsstrahlung and photons with the spectrum of the ROCUS apparatus, a mathematical model of dose kernels of a pencil beam is proposed, which includes decomposition of the dose kernels into components of the primary and scattered doses, approximation formulas and empirical coefficients convenient for integration. The values of empirical coefficients are determined by fitting to the results of the calculation of dose kernels using a combination of the random search method and the nonlinear regression method.

Conclusion: The results obtained in this work will improve the algorithms and increase the accuracy of dose calculation when planning remote therapy with photon beams.

Keywords: photons, pencil beam, dose kernel, bremsstrahlung, radiation therapy, mathematical model, approximation formulas

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Introduction

Model planning methods [1], based on the use of dose kernel for elementary sources of photons, have found wide application in treatment planning systems (TPSs) of distance radiation therapy with photon beams. These dose kernels are the relative spatial distributions of the energy absorbed per unit volume of the water medium near an arbitrary point in space. Their numerical values are usually pre-calculated by the Monte Carlo method. The most popular models are the DPB (Differential pencil beam, also called the “Point spread function” model) [2], and the PB (Pencil beam) [3] model.

Starting from these works [1, 2], the methods of dose kernel (kernel methods) gradually became the most popular in SP of irradiation. They became especially widespread with the advent of 3D dosimetry planning and the development of new technologies and irradiation treatments [1]. Their undoubted advantages are good adaptability to dose calculation in complex inhomogeneous 3-dimensional geometry and high calculation speed. Despite the rapid development of computing technology, which allows in some cases to apply more rigorous methods, interest in these methods and their relevance have not disappeared even now [1].

Improvement of the radiation therapy (RT) equipment and technologies and increasing the requirements for calculation accuracy (total error to the delivered dose < 5 % [1]) of the dose initiated the development of specialized dose kernels intended for use in specific RT technologies. So the development of the method of stereotactic irradiation and

radiosurgery caused the appearance of a number of works in which dose kernel for narrow beams with a circular cross section were proposed, for example, the phenomenological model in [4]. The emergence of the IMRT technology has stimulated the development of dose kernel for the so-called FSPB (finite size PB, a divergent beam of photons with a small square cross section). Such kernel were obtained, for example, in [5]. When it turned out that the dose kernels methods existing at that time in some cases do not provide the required accuracy, in particular when calculating the dose in heterogeneous environments and oblique incidence of radiation on the patient, a new algorithm called AAA (anisotropic analytical algorithm) was created based on the PB model. The theoretical foundation of this algorithm was laid in [6, 7], and its implementation was carried out in the Eclipse SDP in 2009 [8].

The interest in improving the methods of dose kernel does not disappear even now. The progress of computer technology, the development of new technologies for RT and new programs that solve problems of radiation transfer, as well as the improvement of libraries of radiation interaction sections with matter stimulated in some cases the revision of existing data on dose kernel, their determination with less statistical and systematic errors, with more detailed results, and with reference to a specific type of therapeutic setting, for example, [9-11]. In some works, methods for obtaining dose kernels were developed not by calculation, but on the basis of experimental measurements of dose distributions in a water phantom [8,12].

In the majority of studies, dose kernel for photons with a bremsstrahlung spectrum were studied. But there were also works in which dose kernel for monoenergetic sources of photons were investigated. The most detailed information in this direction was obtained in [13, 14]. In these studies, dose kernel were calculated using the Monte Carlo method and a library of dose kernel was created [14] for a large set of monoenergetic sources of photons in DPB and PB geometry in the energy range from 0.1 MeV to 30.0 MeV with an uneven energy step.

The direct use of data on dose kernels in the form of numerical arrays in the dosimetric planning of the RT encounters certain difficulties. The reason is that the strict determination of the dose values at specific points is connected with the numerical calculation of multidimensional integrals (over 3-dimensional space, along the directions of incidence and over the spectrum of the photon beam) [1–3]. At the same time, the dose distribution with preliminary dosimetric planning of RT is calculated at hundreds of thousands of points inside the patient in complex 3-dimensional heterogeneous geometry, and the planner with the help of TPS repeats such calculations many times (and the optimization system hundreds and thousands of times) to select the most optimal treatment plan, changing the number of irradiation fields, the size and shape of the fields, the direction of the beams, etc. The second reason is related to the fact that the spatial dependences of the dose kernel have very high gradients [1, 15], which make it difficult to interpolate numerical data. Therefore, in the practical application of the methods of dose kernel, an important factor is the shape, adequacy and compactness of the ways of representing and interpolating their values. The time and uncertainty of the calculation strongly depends on this. In this regard, the analytical approximation expressions proposed for the bremsstrahlung photon dose kernel DPB and PB in the works [2, 3] turned out to be very useful in calculating the dose from therapeutic beams.

Next, we will focus on the data and mathematical models of PB dose kernel. The most widely used in the literature and in practice is the mathematical model of the PB dose kernel proposed in [3]. In this model, the dose kernels is represented as the sum of the primary dose, which is created by charged particles created during the first interaction of the primary photons with the substance, and the “scattered” dose created by the photons scattered in the medium. The popularity of this model is largely connected with convenient for integration analytical approximation expressions describing the radial distribution of the absorbed energy for the primary and scattered components. The values of the empirical coefficients in [3] are given for continuous bremsstrahlung spectra with a maximum energy of 4, 6, 10, 15 and 24 MeV. According to the authors of [3], the results of calculating the dose kernel of PB according to the proposed approximation formulas agree well with the original data obtained by the Monte Carlo method (the error values were not given), with the exception of the near and far zones in relation to the sources.

For monoenergetic photon sources in PB geometry, approximation formulas were proposed in [13, 14], and also separately for the primary and scattered components of the dose kernels. They had less uncertainty (mean square error $\leq 5\%$) than the approximation formulas of work [3], however, they turned out to be less convenient when calculating the dose in RT through integrating the dosage kernels of the PB into which the therapeutic beam is divided by the irradiated volume.

Thus, it can be stated that by the beginning of the 21st century, there were sufficiently detailed data on the dose levels of PB in the literature. However, the constant increase

in requirements in RT for the reduction of uncertainty in planning and delivering doses often stimulates the return and critical analysis of many previously solved tasks. The use of the method of dose kernel of PB takes place in almost all modern TPS; therefore, problems of uncertainty in their values and convenience of their practical application are regularly raised in the literature. Considering the above, the purpose of this work was a critical analysis of the information currently available in the literature on this area and the creation of new version of the library of PB dose kernels based on new data on interaction cross sections and improved algorithms for calculating radiation transfers.

Material and methods

Earlier a library of dose kernel was created for elementary sources of photons in the form of a differential thin beam (DPB) and a PB [14]. The geometry of these sources and the coordinates of the points of detection are shown in Fig. 1. The term “dose kernels PB” (or, according to the terminology [2], “thin beam kernel”) is the spatial distribution of the relative fraction of the energy of a point monodirectional source of photons normally falling on a semi-infinite water medium and absorbed per unit volume of the medium in the vicinity of an arbitrary point \vec{r} . For water, this is equivalent to the relative distribution of the absorbed dose. In a cylindrical coordinate system with the origin at the point where the PB falls on the medium, the dose kernels will be a function of the photon spectrum, the depth z , and the transverse distance r of the detection point from the PB. Denote this value by $K(E, z, r)$.

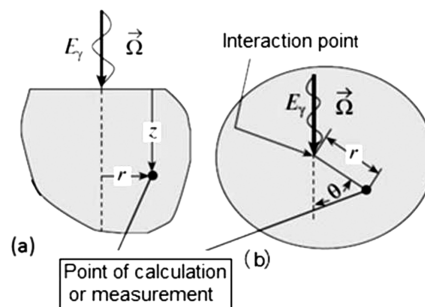


Fig. 1. Geometry of determination of dose kernel for PB (a) and DPB (b)

The dose kernel of DPB were calculated using the Monte-Carlo method using the GEWATER program, which is part of the ELISA complex [16], and for PB using program [17]. In the calculations, the photon interaction cross sections for Storm and Israil [18] were used, the simulation of incoherent photon scattering was carried out according to the Klein–Nishina–Tamm theory, the trajectories of electrons and positrons were modeled using the recommendations summarized in [19], with 5 % energy losses at the step of a charged particle. A detailed description of the algorithms for modeling charged particles used in [14] is given in [20]. Dose kernel in works [2, 3] and in most other publications of that time were also determined by the Monte Carlo method using the well-known EGS4 code [21, 22], in which the trajectories were simulated on the basis of approximately the same approaches described in [19].

Over the past more than 20 years since then, the refinement, revision and improvement of both the databases on the cross sections for the interaction of photons and charged particles with matter, and the algorithms for modeling the transfer of ionizing particles in matter have occurred. Especially great progress was made in the field of modeling the trajectories of charged particles, which is partially reflected in [23, 24]. An important factor is also the impressive pro-

gress of computing, which now makes it possible to carry out calculations with much smaller statistical uncertainties than before.

Considering these moments in the present work, the EGSnrc code [25], which is a substantially improved version of the EGS4 code, was chosen as a settlement tool. In particular, the modeling of the transport of low-energy photons and electrons has undergone significant modification, taking into account the coupling of electrons in an atom and the processes of relaxation of atoms after Compton scattering and photoabsorption of photons, etc. The EGSnrc complex was repeatedly tested and verified using experimental data (for example, in [26–28]). At present, it is in some sense a “gold standard” in calculating the transfer of electrons and photons in the low and medium energy region, with which the results of calculation by other programs (MCNP, PENELOPE, GEANT4, etc.) are compared, implementing the Monte Carlo method. We give for example the work [29]. At the same time, EGSnrc has a friendly interface and high speed.

In this work, PB dose kernel were calculated for water using the EGSnrc code in cylindrical geometry for monoenergetic and bremsstrahlung photons, as well as photons with the spectrum of the ROKUS therapeutic device with the Co-60 radionuclide. The components of the primary and scattered dose were determined separately.

As noted above, A. Ahnesjo et al in [3] proposed a mathematical model for dose kernel of PB photons for a number of bremsstrahlung spectra in the interval from 6 to 18 MV, including an approximation expression that is convenient for analytical integration over the irradiated volume at 3-dimensional dose calculation in RT. This formula has the following form:

$$K(z, r) = (A_z \cdot e^{-a_z \cdot r} + B_z \cdot e^{-b_z \cdot r}) / r, \quad (1)$$

where A , a , B , b are empirical coefficients depending for a given photon spectrum on the depth of the calculation point. Their values for several spectra of the bremsstrahlung beams were received in [3] using the nonlinear least squares method by fitting the Monte Carlo method to the results of calculating the PB dose kernel.

An important feature of the model is that, according to the authors [3], the first term in the formulas approximately describes the contribution to the dose kernel from the primary component (the dose from the electrons produced by the interaction of the primary photons with water), and the second term – the contribution of the scattered component (dose from photons scattered in water). Note that the authors of [3] do not give the error values for describing the results of the calculation of dose kernel and their individual components according to the proposed model. However, from the graphical comparisons given in the text of [3], it can be concluded that the discrepancies in the near and far zones with respect to the incident point of the PB on water reach 20–25 %. This conclusion is confirmed by the analysis carried out in [14]. Alternatively, in [14], approximation expressions were proposed that describe the spatial distributions of the individual components of the dose kernel with greater accuracy. But these expressions were inconvenient for numerical calculations of doses in RT.

Taking into account these circumstances, a more adequate mathematical model of the photon PB dose kernels for the bremsstrahlung spectra with a maximum energy of 6.0, 10.0, 18.0 MeV and for the spectrum of the ROKUS therapeutic machine with the Co-60 radionuclide is developed in this work. In this model, the strengths of A. Ahnesjo model [3] are preserved, namely, the separation of the dose kernels into two components in accordance with their different spa-

tial dependencies, and an analytical form of approximation expressions that is convenient for integration. However, to approximate the spatial dependence of the individual components with higher accuracy (uncertainty $\leq 5\%$), not one but several members are used. Thus, the dose kernel is represented as the sum of the primary and scattered components:

$$K(E, z, r) = K_p(E, z, r) + K_s(E, z, r). \quad (2)$$

Further, for brevity, the variable E will be omitted, but implied. For analytical approximation of the radial dependence of each PB component, the following analytical expression was used:

$$K_j(z, r) = \sum_{i=1}^{N_j} C_{j,i}(z) \cdot e^{-k_{j,i}(z) \cdot r} / r, \quad (3)$$

where $j = p$ or s for the primary and scattered components, respectively; N_j is the number of terms of the sum depending on the quality (spectrum) of the beam and the type of component; C_i and k_i are empirical coefficients depending on depth for PB and on angle for DPB, the values of which were determined by the non-linear regression method in combination with the random search method through fitting the calculation results using formula (3) to the Monte-Carlo calculation results. The technique used to find empirical coefficients was proposed earlier in [30] and described in more detail in [31]. For the bremsstrahlung spectra with maximum energy of 6 and 18 MeV, it turned out that two terms in each component were sufficient; for the spectrum of the ROKUS apparatus and for 10 MeV the number of members in the row for the scattered component had to be increased to 4.

In practice, the integral form of the PB dose dose is also often useful:

$$\begin{aligned} K_{\text{int}}(z, R) &= 2\pi \int_0^R r \cdot K(z, r) \cdot dr = \\ &= 2\pi \sum_{i=1}^N \frac{C_i(z)}{k_i(z)} (1 - e^{-k_i(z) \cdot R}), \end{aligned} \quad (4)$$

since its value is numerically equal to the dose created at depth z in a water phantom on the axis of a disk mono directional source of radius R . As can be seen from formula (4), the value of $K_{\text{int}}(z, R)$ is easily determined in the framework of the proposed model. For the sake of definiteness, we will further call expression (3) the differential form of the PB dose kernel.

Results and discussion

In this paper, using the EGSnrc code in cylindrical geometry, we calculated dose kernel of PB in water for monoenergetic photons in the energy range 0.25–19.75 MeV with 0.5 MeV increments, brake photons with maximum energies 4.0, 6.0, 10.0, 15.0 and 18.0 MeV with a spectrum of therapeutic apparatus ROKUS with radionuclide Co-60. Dose kernel are defined in a water phantom for depths of 0.5–40 cm with a step of 0.5 cm and for radial distances of 0.02–46 cm with an uneven grid. The components of the primary and scattered dose were calculated separately. The statistical uncertainty for the primary component was less than 1.0 %, for the scattered one, not higher than 2.0 % except for certain points located at large radial distances and at the same time at shallow depths in a water phantom. The results obtained are included in a single multidimensional array in the mathematical package MATLAB and are also presented in the form of a collection of txt-files for each value of the energy of PB photons.

We first compare the results obtained in this work with the results of [3] and [14]. In [3], tables with the values of dose kernel obtained by the Monte Carlo method are not given, and there are only graphical demonstrations comparing the values of dose kernel calculated by the Monte Carlo method and determined by formula (1). Therefore, the possibility of direct comparison of the numerical values of the kernel with the results of this work is absent. But for the spectrum of the bremsstrahlung photons with maximum energy of 18 MeV, the values of empirical coefficients for formula (1) are given, and with these calculations the comparison is made in Fig. 2 and 3. As can be seen from fig. 2 and 3, the difference between the results of work [3] and the present work becomes very significant in the near and far zones.

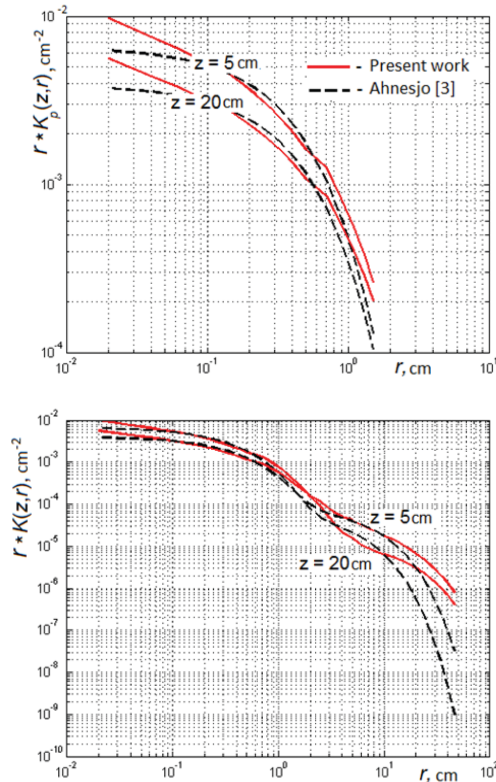


Fig. 2. Comparison of the results of the calculation of the radial distributions of the primary component and the total value of the dose kernel using the formula (1) with the empirical coefficients of work [3] and the results of the Monte-Carlo calculation in the present work for a PB of the bremsstrahlung spectrum with maximum energy of 18 MeV at different depths in a water phantom

A significant difference is also observed when comparing the results of this work with the data on dose kernel included in the library [14]. Examples of such comparisons are given in fig. 4 and 5. From fig. 4 and 5, the difference between the data increases with increasing distance from the PB axis. This may be partly due to the insufficient number of trajectories, which were simulated in [14] when calculating for such sharply decreasing distributions with increasing radius (Fig. 4a). At the same time, it is known that when calculating functionals in the field of radiation transfer by the Monte Carlo method in case of insufficient statistics, the result is often underestimated. In [14], about 10^6 photon trajectories were simulated for each depth. In the present work, after studying the convergence of the calculation results, the number of trajectories was increased to 10^8 , which naturally very significantly improved the statistical accuracy of the calculation.

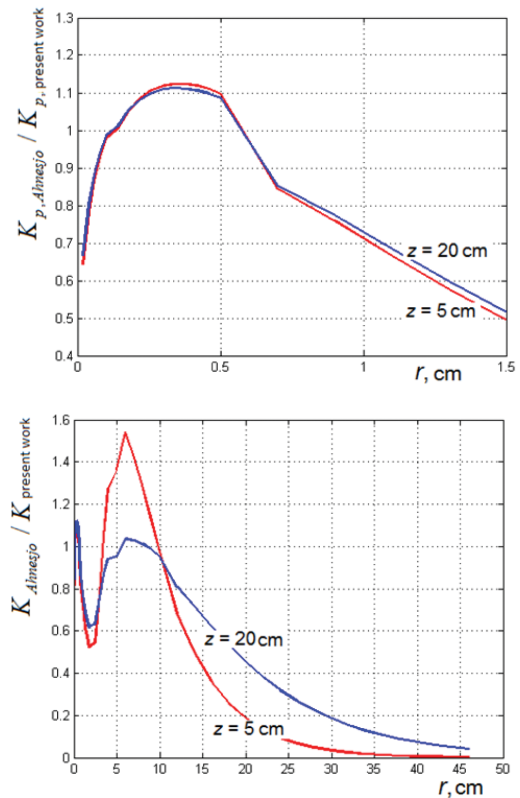


Fig. 3. Dependence of the relationship of the calculation results of the primary component and the total value of the dose kernels using formula (1) with empirical coefficients of work [3] and the results of the Monte Carlo calculation for PB of the bremsstrahlung spectrum with maximum energy of 18 MeV at different depths in the water phantom from the transverse distance to the axis PB

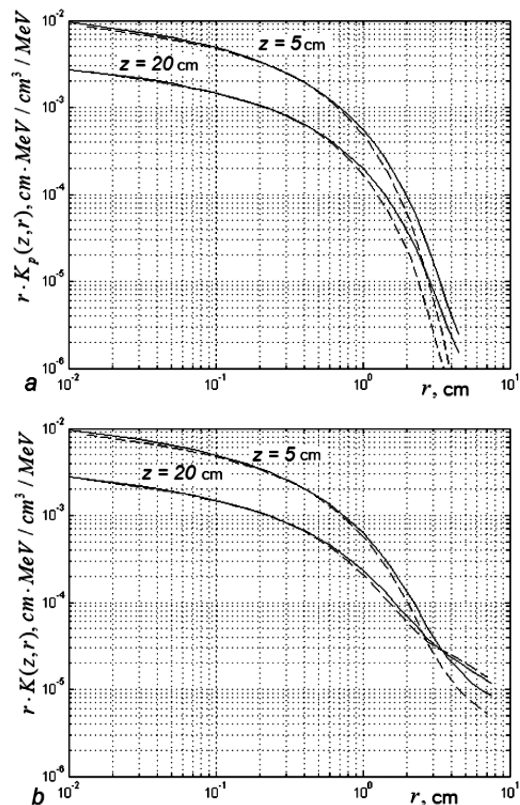


Fig. 4. Comparison of the calculation results of the PB dose kernel obtained in the present work by the Monte-Carlo method (—) and in [14] (---) for the primary component (a) and the total value of the dose kernel (b) at different depths water phantom. Data for $z = 20$ cm multiplied by 0.5

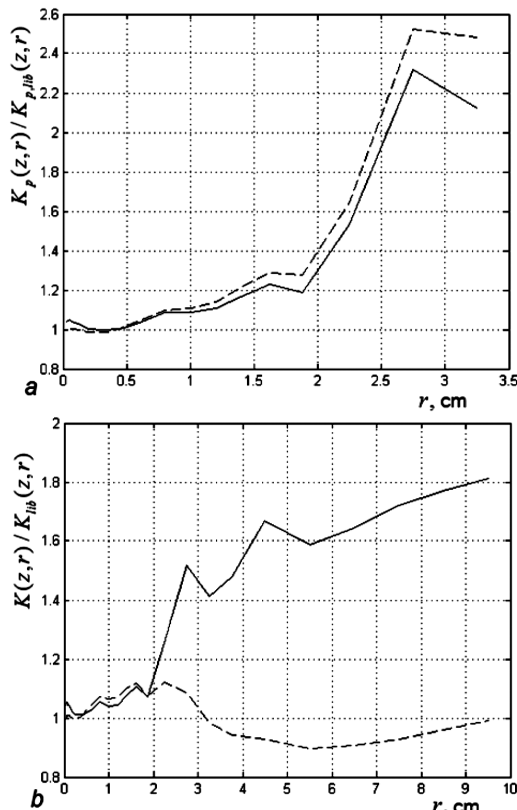


Fig. 5. Dependence of the ratio of the values of PB dose kernel obtained in the present work and in work [14] for the primary component (a) and the total value of dose kernel (b) at depths in a water phantom of 5 cm (—) and 20 cm (---)

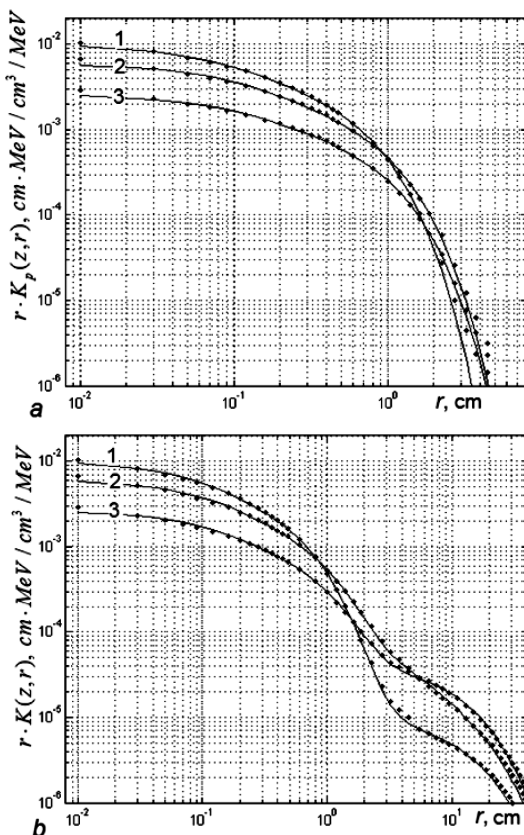


Fig. 6. Comparison of the radial distributions of the primary component (a) and the total value (b) of the dose kernels of the PB photons of the bremsstrahlung spectrum with maximum energy of 18 MeV obtained by the Monte-Carlo method (•) and by the formulas (2) and (3) (—) in water phantom at depths of 3 cm (1), 15 cm (2) and 40 cm (3)

As noted above, in many practical cases it is preferable to use not tables with the numerical values of the PB dose kernel, but convenient analytical approximations. Such a task for a number of photon PB spectra was performed in the present work. The formula (3) was taken as an approximation expression. The empirical coefficients in formula (3) were determined by fitting the calculation results using formula (3) to the data obtained by the Monte Carlo method. For this, a combination of the random search method and the nonlinear regression method was used, which was described in more detail in [31]. The results of approximation of the PB photon dose kernel for the bremsstrahlung spectrum with a maximum energy of 6.0 MeV and the spectrum of the ROKUS therapeutic apparatus charged with the Co-60 radionuclide were published in [30, 32, 33]. Therefore, we dwell here on the results of approximation of the PB dose kernel for the bremsstrahlung spectrum with maximum energy of 18 MeV, the form of which was taken from [34]. For this spectrum in the series of formula (3) it turned out to be sufficient to take two terms for each component. Some results for the values of empirical coefficients are presented in Table 1 and 2.

The average uncertainty of the approximation using the expressions (2) and (3) of the Monte Carlo calculation results in the region that is significant for calculating the dose was < 5%. Uncertainty increases to 10% or more in areas where the dose kernel value is much smaller (two orders of magnitude or more) than for small radii. In fig. 6, as an example, a comparison is given of the radial distributions of the dose kernels of PB photons with 18 MV bremsstrahlung spectrum obtained by the Monte Carlo method and using formulas (2) and (3).

Table 1

The values of empirical coefficients of approximation by the expression (3) data for the primary component of the dose kernels of PB photons of the bremsstrahlung spectrum with maximum energy of 18 MeV, obtained by the Monte Carlo method

Depth, cm	C ₁	C ₂	k ₁	k ₂
2	5.5124e-3	5.2650e-3	2.9966e+0	1.3467e+1
3	4.9309e-3	5.2331e-3	2.3901e+0	1.2172e+1
5	3.8757e-3	5.1293e-3	1.9108e+0	9.6820e+0
7	3.4268e-3	4.7814e-3	1.7960e+0	8.9569e+0
10	3.0927e-3	4.2107e-3	1.7638e+0	8.7751e+0
15	2.6499e-3	3.4033e-3	1.7297e+0	8.6240e+0
20	2.2845e-3	2.7821e-3	1.7027e+0	8.5898e+0
25	1.9749e-3	2.2872e-3	1.6795e+0	8.5214e+0
30	1.7209e-3	1.8998e-3	1.6647e+0	8.6835e+0
35	1.4950e-3	1.5887e-3	1.6435e+0	8.7199e+0
40	1.3126e-3	1.3326e-3	1.6323e+0	8.9490e+0

Note: The average deviation of dose kernels primary component calculation according to formulas (3) from the results of its simulation by the Monte Carlo method is less than ± 5%

Table 2

The values of empirical coefficients approximation by the expression (3) data for the scattered component of the dose kernels of PB photons of the bremsstrahlung spectrum with maximum energy of 18 MeV, obtained by the Monte Carlo method

Depth, cm	C ₁	C ₂	k ₁	k ₂
2	9.2584e-6	7.7444e-5	8.1596e-2	1.3790e+0
3	1.0994e-5	9.1349e-5	8.3088e-2	1.0421e+0
5	1.4252e-5	9.8921e-5	8.5089e-2	7.1960e-1
7	1.7308e-5	9.6510e-5	8.6407e-2	5.5996e-1
10	2.1531e-5	8.7277e-5	8.7709e-2	4.2867e-1
15	2.7713e-5	6.8693e-5	8.9207e-2	3.1519e-1
20	3.3147e-5	5.0689e-5	9.0594e-2	2.5320e-1
25	3.8477e-5	3.3850e-5	9.2384e-2	2.1374e-1
30	4.4814e-5	1.7315e-5	9.5144e-2	1.8552e-1
35	-6.3079e-7	5.3997e-5	5.6033e-2	9.7765e-2
40	-2.3062e-9	4.7343e-5	4.0492e-2	9.2095e-2

Note: The average deviation of dose kernels scattered component calculation according to formulas (3) from the results of its simulation by the Monte Carlo method is less than ± 5%

Conclusion

Thus, a new version of the library of PB dose kernel of photons in water, differing from the previous library [14], has been used in calculating a more advanced description and modeling of physical processes of interaction between photons and charged particles with matter [23, 25], with more adequate data by the interaction cross sections [23] and by significantly smaller values of the statistical uncertainties of the results obtained. The library includes data for monoenergetic photons in the energy range of 0.25–19.75 MeV in 0.5 MeV increments, data for bremsstrahlung photons with a maximum energy of 4.0, 6.0, 10.0, 15.0, 18.0 MeV, and data for the spectrum of the ROKUS therapeutic machine. Depths in water from 1.0 to 40 cm with a step of 0.5 cm and along the radius from 0.02 to 46.0 cm with an uneven grid were studied. Comparison of the results with the data obtained in [3, 14] showed significant discrepancies, especially for large distances in depth and in radial distance from the

axis of the PB. The paper proposes a more accurate mathematical model for the primary and scattered components of PB dose kernel, including approximation expressions for calculating the component values, and empirical model coefficients for a number of bremsstrahlung and photon spectra of the ROKUS therapeutic machine are defined. The average deviation of the calculation results for dose kernels according to formulas (2) and (3) from the results of dose kernels simulation using the Monte Carlo method is less than $\pm 5\%$. This gives reason to believe that the uncertainty in calculating the dose using the pencil beam method using the results of calculation and approximation of dose kernels, obtained in this work, will have an error of no more than 5%.

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