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Implementation and validation of the method for the energy spectra reconstruction of electron beams generated by the AQURE mobile accelerator

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ABSTRACT

Background: The energy spectrum is the main component of the Monte Carlo model of the electron beam. One possible method to obtain it is a backward reconstruction from the measured depth dose distribution, owing to solving the inverse first-degree Fredholm integral equation with appropriate regularisation. This study aimed to reconstruct and validate energy spectra for mobile intraoperative accelerators.

Materials and methods: The Geant4 package was used to simulate percentage depth dose (PDD) distributions. The microDiamond detector and the BeamScan water phantom were used to measure PDD. 160 PDDs were simulated for quasi-monoenergetic beams with energies from 0 to 20 MeV for a 10 cm diameter applicator. Using the simulated and measured PDDs, energy spectra were reconstructed for all available nominal energies by solving the inverse Fredholm equation. A single Gaussian peak was used as a reference solution, and the regularisation parameter λ was set to 0.05. Obtained spectra were used to simulate PDD for 5 and 6 cm applicators and compared with the measurements.

Results: Simulated and measured PDDs were compared using the gamma analysis method with 2% DD and 2 mm distance to agreement (DTA) criteria. Measured and simulated PDDs agree perfectly for the 4 MeV beam. For higher energies, the PDDs agree at all depths except for depths less than 2 mm.

Conclusion: The numerical solution of the inverse Fredholm equation with Tikhonov regularisation using simulated annealing optimisation is a reliable method to reconstruct the energy spectrum for electron beams produced by mobile intraoperative accelerators.

Key words: IOERT; Monte Carlo; dual annealing

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Introduction

Intraoperative electron beam radiotherapy (IOERT) is a radiation therapy procedure performed during surgery and used to irradiate the target area, which is a neoplastic tumour or the area of tissues defined as the tumour bed removed during the operation [1–3].

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The AQURE is a mobile accelerator dedicated to IOERT, and it is currently being developed by the Polish National Center for Nuclear Research (NCBJ) [4, 5]. This accelerator can generate electron beams with energies ranging from 4 MeV to 12 MeV. Due to the wide range of available applicators, the diameters of the circular fields are from 5 cm to 10 cm. The dose rate is 10 Gy per minute, allowing the dose to be delivered in less than 2 minutes.

Along with constructing the machine, its model for the Monte Carlo (MC) simulation is being created. The energy spectrum is an essential component of any electron beam model. Due to the specific construction requirements of mobile accelerators dedicated to IORT (i.e., no bending magnets as energy selectors), the electron beam energy spectrum has a more complex shape than the spectra obtained by the conventional accelerators [6–8].

Our previous study presented an approach to backward spectrum reconstruction from the measured data based on solving the inverse first-degree Fredholm integral equation with appropriate regularisation (i.e. Tikhonov regularisation and the Dual Annealing optimisation method) [9], as described in "Materials and Methods". The aim of that study was to determine the optimal value of the Tikhonov regularisation parameter for determining the spectrum of the electron beam produced by an IOERT mobile accelerator. While it succeeded in finding the optimal value of the regularisation parameter, the study had a purely simulation nature. Continuing our research, here we present our method for practical implementation and validation of measured data obtained on the AQURE mobile accelerator. The aims of the current study are (1) reconstruction of the original energy spectra for electron radiation beams with nominal energies of 4, 6, 9, and 12 MeV for the AQURE intraoperative accelerator and (2) validation of the reconstructed energy spectra by comparing the percentage deep doses (PDDs) generated by using the MC method with the PDDs obtained during measurements.

Material and methods

Construction of a model of a beam-forming system

Based on the technical documentation of the AQURE intraoperative radiotherapy device received from the manufacturer, the exact geometry of the beam-forming system was reconstructed [4, 5]. The reconstruction was performed in the Geant4 v.11.01.p01 package [10]. Figure 1 shows a visualisation of the created model with the key elements of the system highlighted.

The simulation included all the elements through which the generated electron beam passes. The elements supporting the individual components and the cover elements were also included. The first and second scattering foils, the set of two ionisation chambers, and the applicators forming the field size were reproduced with particular accuracy. During the reconstruction, the materials of the individual elements of the beam-forming system were taken into account. The model includes three exchangeable applicators of different sizes, enabling a circular field shape with diameters of 5, 6 and 10 cm, respectively.

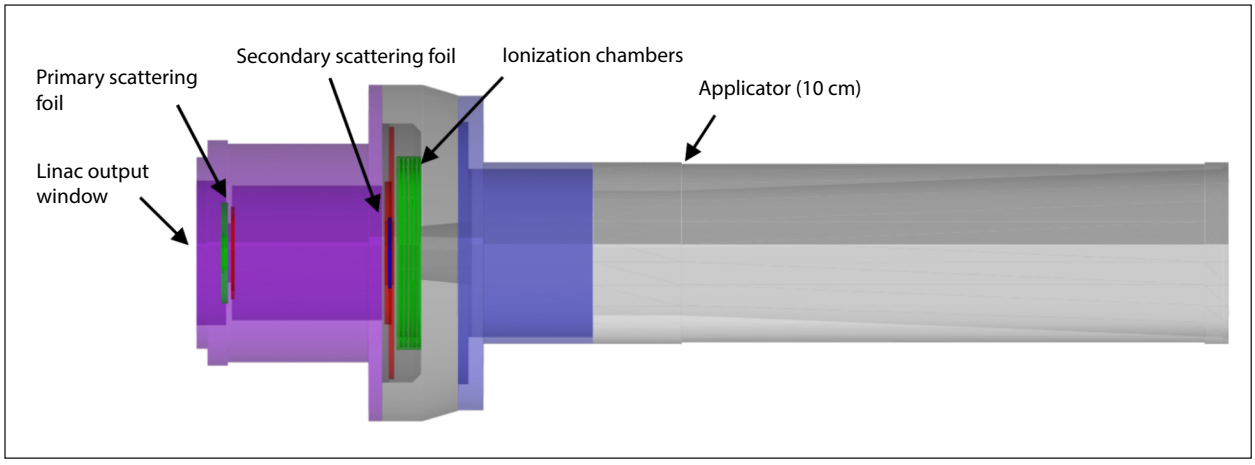

Figure 1. Visualisation of the Geant4 model with key components of the accelerator beamforming structure highlighted

The beam-forming system's model was used in the Monte Carlo (MC) simulation. In the first stage of the simulation, an applicator with a diameter of 10 cm was used to generate quasi-monoenergetic beams needed in the energy spectrum reconstruction process. In the next steps, the reconstructed energy spectra were used to simulate the PDDs for all applicators (5, 6 and 10 cm), which were, in turn, compared with the measured PDDs. The spectrum generation and verification procedures were performed for each of the four nominal energies, i.e. 4, 6, 9 and 12 MeV available on the AQURE device.

Simulation of monoenergetic depth dose distributions

In order to solve the inverse Fredholm equation, a total of 160 quasi-monoenergetic PDD distributions were simulated, the energies of which ranged from 0 MeV to 20 MeV. For each quasi-monoenergetic PDD distribution, the initial energy of electrons was uniformly distributed in the range:

$$E =< n * 0.125\ MeV, (n+1) * 0.125 MeV) \quad (1)$$

where n = 0, 1, …, 159.

10^9 electrons emitted from the primary source were used to obtain each distribution. For the simulation, a model of a cubic water phantom was placed so that the end of the applicator was directly above the water surface. In the phantom, cylinder-shaped detectors with a diameter of 5.5 mm and a height of 1 mm were placed in the beam axis, one above the other on a section from the surface to a depth of 20 cm. During the simulation, these detectors recorded the dose deposited in them, which allowed the generation of graphs showing PDD distributions for beams with a very narrow energy range (quasi-monoenergetic beams). Based on the quasi-monoenergetic depth distributions generated in this way, it was possible to determine the PDD distribution for a beam with any shape of the energy spectrum in the range from zero to 20 MeV as a weighted sum of distributions coming from monoenergetic beams [11, 12].

Measurement of the percentage depth doses

The PDD curves were measured in a BeamScan water phantom (PTW-Freiburg, Germany) using a solid-state synthetic crystal diamond microDiamond detector (PTW-Freiburg, Germany). The microDiamond detector was chosen due to dose measurement and no need for recalculation from the ionisation curve, which was a problem due to non-standard conditions. The measurements for circular fields were performed for 4, 6, 9, and 12 MeV electron energies generated by the AQURE accelerator. The PDDs were collected at a nominal distance (60 cm) between the source and the water surface (SSD). The detector was placed parallel to the beam's central axis (CAX), and the measurements were performed along the CAX. The geometry of the measurements directly corresponded to the geometry used in the MC simulations. Due to measurement geometry that prevents the use of the second (reference) detector during measurements (i.e. the applicator, from one side, was fixed to the gantry and, from the other side, was in direct contact with the surface of water), the measurements were repeated three times and averaged [13].

The 3D printed thin-walled and transparent applicators defined the circular electron fields with 5, 6 and 10 cm diameters. The applicators are biocompatible, transparent materials with a 1.19 g/cm^3 density. The measurements were analysed with PTW Mephysto software v.3.4 (PTW-Freiburg, Germany). All PDDs were normalised to the maximum dose.

The microDiamond detector was chosen because of high dose linearity (AQURE dose rate is 10 Gy/min) and low energy dependence [14, 15]. The water-to-carbon mass collision-stopping power ratios are almost constant in the range of electron energies from 1 MeV to 20 MeV for this detector [16]. This enables a direct comparison of the measurements with the MC calculations without any corrections. Measurements for an applicator with a diameter of 10 cm were used to reconstruct the energy spectra (i.e. for 4, 6, 9, and 12 MeV nominal energies), and the remaining measurement data were used for verification.

Energy spectrum reconstruction

The Dual Annealing method with Tikhonov regularisation was used to perform backward reconstruction of the energy spectrum. Our previous work thoroughly described and verified this method [9].

The distribution of the percentage deep dose D(z) for an electron beam with a certain energy

spectrum Φ(E) can be written as a composite of the depth distributions D(z,E) derived from monoenergetic beams:

$$D(z) = \int_{min}^{max} D(z,E)\Phi(E)dE \quad (2)$$

Such equation is known as the first-degree Fredholm integral equation, and after discretization, it can be written as [11, 12]:

$$D(z_j) = \sum_i D(z_j,E_i)\Phi(E_i)\Delta E_i, \quad (3)$$

where: z_j - the following depths, E_i - consecutive energy values of mono-energetic beams, ΔE_i - width of the interval between the energies E_i and E_{i+1}.

The inverse problem of the integral Fredholm equation, i.e. determination of the spectrum $\Phi(E_i)$, based on the knowledge of $D(z_j)$ and $D(z_j,E_i)$, is ill-conditioned. Therefore regularisation is needed to define additional conditions resulting from apriori information about the nature of the problem under study. One of the well-known regularisation methods for solving first-degree Fredholm's integral equations is Tikhonov regularisation [17], where an additional term extends the objective function of the original problem, called the solution norm:

$$\lambda^2 \left|\left|L(\Phi - \Phi_0)\right|\right|_2^2 \quad (4)$$

where λ is the regularisation parameter, L - is the regularisation matrix, and Φ_0 - is the reference solution, whose features should have the solution we are looking for.

Our study used a single Gaussian peak as a reference solution. The regularisation parameter λ was set to 0.05 for all nominal energies based on our previous work [9].

Due to the probabilistic nature of the method, 50 repetitions of the optimisation process were performed for each reconstructed spectrum. Among them, 10 were selected for the best match between the simulated and measured PDD distributions. The final spectra were determined on their basis.

Verification of reconstructed energy spectra

The reconstructed spectra were applied to the accelerator model generated in the Geant4 application. For each of the four nominal energies (i.e. 4, 6, 9 and 12 MeV), three percentage depth dose distributions were determined, one for each of the available applicators (i.e. diameters of 5, 6, and 10 cm). The arrangement of detectors in the phantom was the same as when determining the distributions for monoenergetic beams. 1E10 electrons emitted from the primary source were used to obtain each distribution.

We used the gamma analysis method to compare the PDD distributions obtained using the reconstructed spectra with the measured ones [18]. The analyses were performed in global mode with the criteria of 2% as the acceptable dose difference (DD) and 2 mm as the acceptable distance to agreement (DTA). The analyses were performed without any dose threshold to enable analysis in the contamination area of the PDD curves where the doses are lower than 1% of the maximum dose. The valid results of the gamma analysis range from 0 to 1. Results higher than 1 are invalid, i.e., the analysis criteria were exceeded.

Results

For the purposes of spectrum reconstruction, 160 PDD distributions were simulated for quasi-monoenergetic beams with energies from 0 to 20 MeV. The simulation was performed for an applicator with a diameter of 10 cm. The time needed to obtain the PDD distribution for a single quasi-monoenergetic beam ranged from 7 hours for the 0.125 MeV quasi-monoenergetic beam to 14 hours for the 20 MeV beam. Simulations were carried out in parallel on five computers (dual Intel Xeon E5 2.4 GHz, 32 GB RAM each). The total time needed to simulate the PDD distributions for all 160 quasi-monoenergetic beams was approximately two weeks.

Figure 2 shows a comparison of measured (black line) and simulated (blue circle dots) PDDs. Both measured and simulated PDDs were obtained for an applicator with a diameter of 10 cm. The simulated PDDs were created as a result of energy spectra reconstruction, aiming to optimally match the weighted sum of distributions coming from quasi-monoenergetic beams to the measured PDD.

Figure 2 also highlights the results of the gamma (red star dots) analysis used to determine the match between the measured and simulated PDD. The best fit was obtained for the lowest nominal energy, i.e.

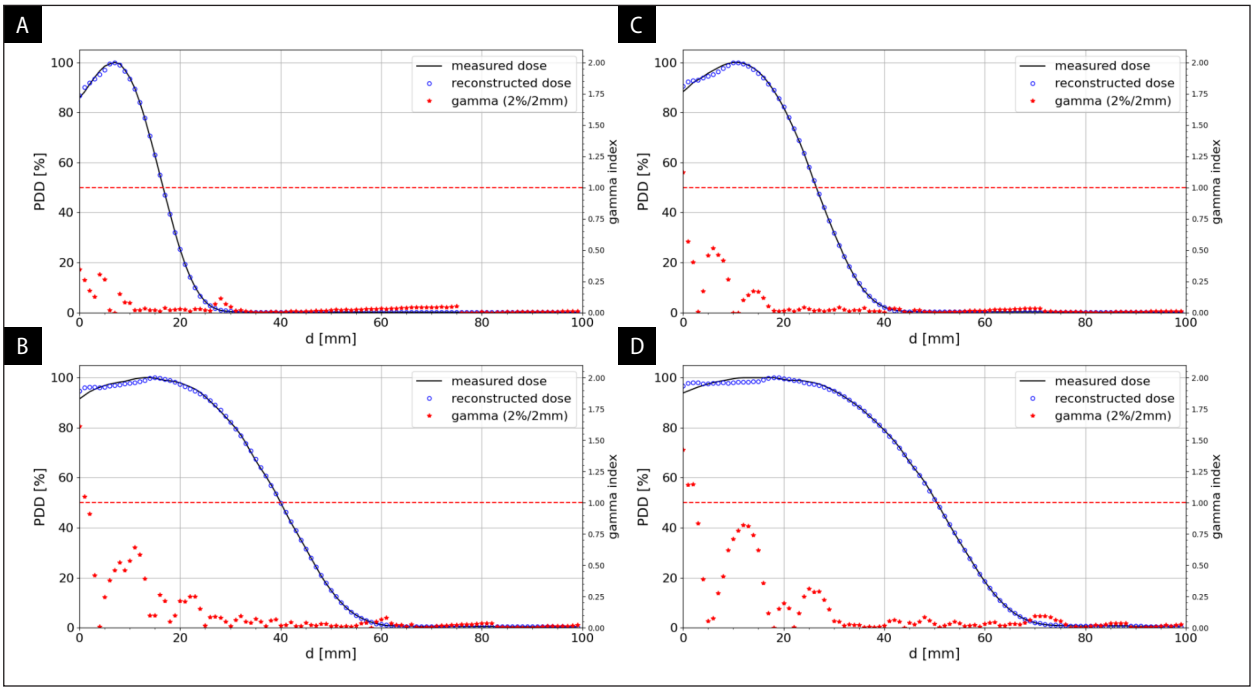

Figure 2. Comparison of the simulated (blue circle dots) and measured (black line) percentage depth doses (PDD) for the beams collimated by a 10 cm applicator and with nominal energies equal to 4 MeV (**A**), 6 MeV (**B**), 9 MeV (**C**) and 12 MeV (D) Results of the gamma analysis (red star dots) were obtained for the criteria of 2 % (dose difference) and 2 mm (distance-to-agreement) and examined in the global mode without any dose threshold.

4 MeV (Fig. 2A). For higher energies, i.e. 6 MeV, 9 MeV, and 12 MeV (Fig. 2B–D), the discrepancies between the measured and simulated PDD increase with the increase in energy and are greatest for the nominal energy of 12 MeV (Fig. 2D). This applies especially to the dose build-up area. However, it should be noted that most of the gamma analysis results are correct. Incorrect results (values > 1) were obtained only at a few measurement points located, respectively, on the surface (0 mm) for an energy of 6 MeV (Fig. 2B) and just near the surface (up to 2 mm deep) for an energy of 9 MeV (Fig. 2C) and 12 MeV (Fig. 2D).

Figure 3 shows the energy spectra obtained as solutions of the inverse Fredholm equation (eq. 3) that best matched the measured PDDs for beams with nominal energies of 4 MeV (Fig. 3A), 6 MeV (Fig. 3B), 9 MeV (Fig. 3C) and 12 MeV (Fig. 3D). The value of the most probable energy (position of the dominant peak) is 5.5 MeV, 8.6 MeV, 11.7 MeV and 14 MeV, respectively, for nominal energies of 4 MeV, 6 MeV, 9 MeV and 12 MeV.

The obtained spectra (Fig. 3) were used to simulate PDDs for beams collimated by 5 cm and 6 cm applicators. The simulations were performed for all nominal energies. Figure 4 shows the comparison of measured PDDs and simulated PDDs and the corresponding gamma analysis results. The graphical presentation of Figure 4 is analogous to the presentation of Figure 2.

Discussion

The experiment confirms the possibility of reproducing the measured PDD distribution on the basis of artificially generated monoenergetic beams and energy spectra deduced from solving the inverse Fredholm equation. The reconstruction was performed for beams formed by an applicator with a diameter of 10 cm. The PDDs reconstructed in this way reproduced the measured PDDs well. Significant discrepancies between the reconstructed and measured PDDs detected by the gamma method concerned a few measurement points located on the surface (0 mm) and just near the surface (up to 2 mm deep) of the water. These discrepancies result from the uncertainty of measurements in this area [19] and - in this particular experiment - the inability to effectively become independent from dose rate fluctuations during the emission of

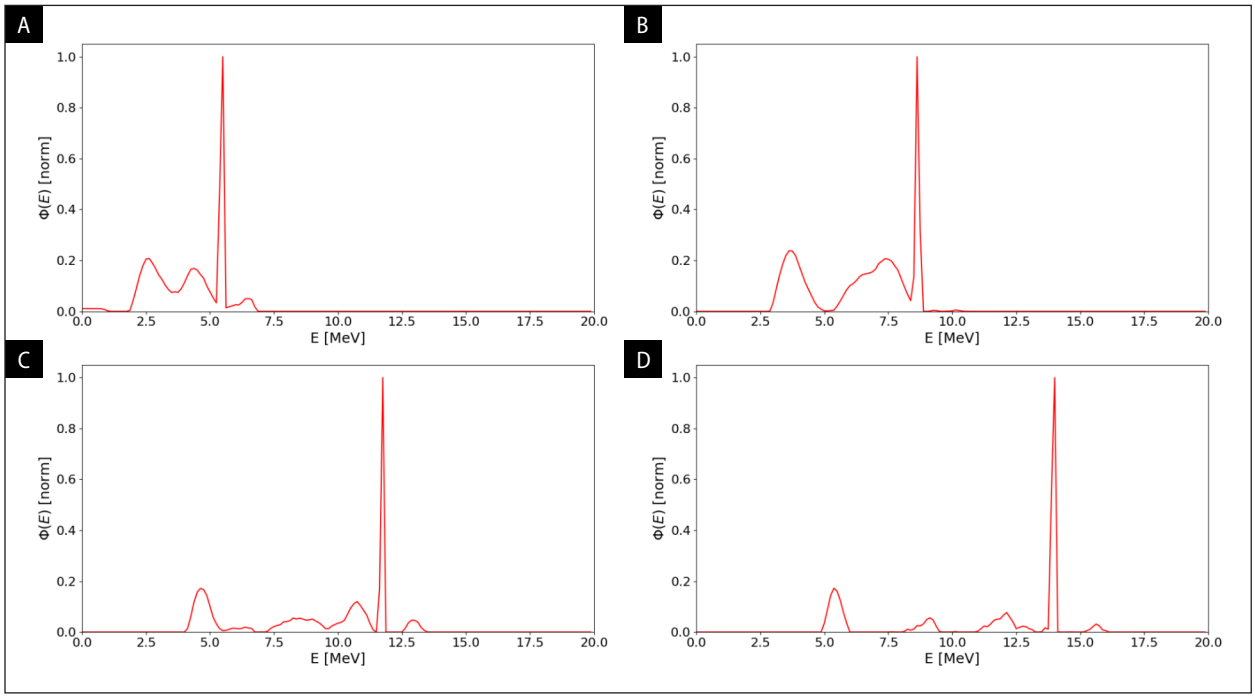

Figure 3. Reconstructed energy spectra for beams collimated by a 10 cm applicator and with nominal energies equal to 4 MeV (**A**), 6 MeV (**B**), 9 MeV (**C**) and 12 MeV (**D**)

electron radiation resulting from the impossibility of using a reference detector [20] which is caused by the design and placement of the applicator that forms the shape of the radiation beam during measurements.

While the absence of the reference detector can be avoided by multiple repetitions of measurements [13], which was done, the dose measurement in the build-up region or at the surface can still deviate by over 10% [21]. One of the possible reasons is the challenges of beam modeling in the build-up region [22]. Although the measurement detector used in the experiment has good dosimetric characteristics, the surface measurements were possible only when the top of the detector housing protruded 1 mm above the water surface due to the effective measurement point being located at a depth of 1 mm in the detector [23]. This known fact negatively affects the accuracy of the surface or near-surface measurements [24].

The values of the DD and DTA parameters used in the gamma analysis when comparing the reconstructed and measured PDDs were dictated by the geometry of the measurement system used during the MC reconstruction. They were selected based on literature data [25].

The reconstruction of energy spectra was possible based on the reconstructed PDD distributions for beams formed with an applicator with a diameter of 10 cm. Figure 3 shows that in the obtained energy spectra, in addition to the dominant Gaussian peak, there are several smaller peaks representing energy ranges other than the most probable energy. This is a different situation than in the case of energy spectra obtained for electron radiation beams generated by conventional therapeutic accelerators, where there is usually only a single Gaussian peak [26]. These differences are caused by the different constructions of conventional and mobile (IOERT) accelerators. The IOERT accelerators have no bending magnets as energy selectors in their heads. Hence, the energy spectrum of the electron beam produced by mobile accelerators has a more complex shape.

While the exact energy spectra of the AQURE accelerator are not known, a tail to the left of the main peak going towards low energies is expected, as shown in calculations using the General Particle Tracer code [27]. The method proposed here produces energy spectra with non-negligible components at energies smaller than the energy of the dominant peak. It shall be noted, however, that

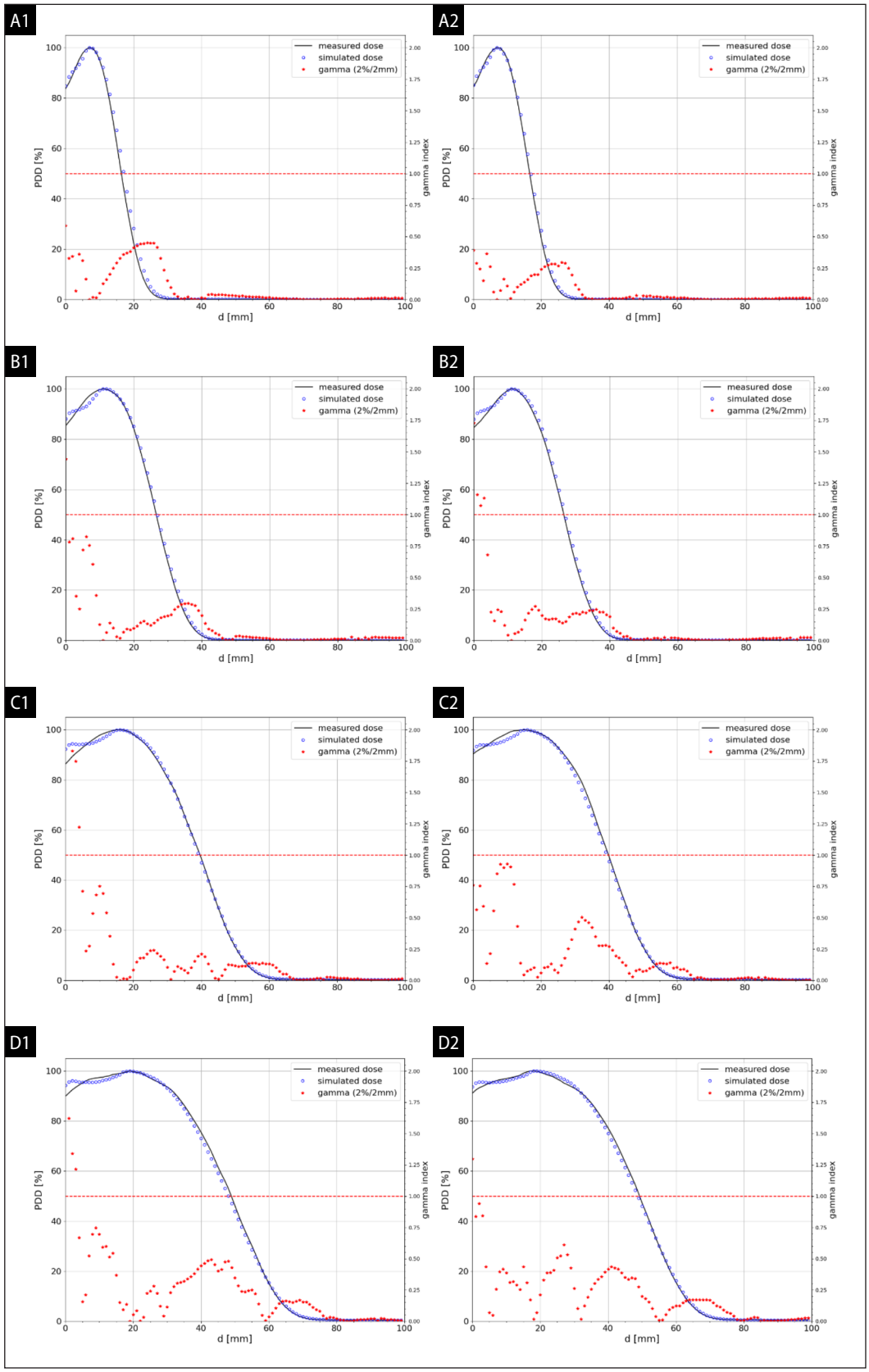

Figure 4. Comparison of the simulated (blue circle dots) and measured (black line) percentage depth doses (PDD) for the beams with 4 MeV (**A**), 6 MeV (**B**), 9 MeV (**C**) and 12 Mev (**D**) nominal energy and collimated by 5 cm (A1, B1, C1, D1) and 6 cm (A1, B1, C1, D1) applicator. Results of the gamma analysis (red star dots) were obtained for the criteria of 2 % (dose difference) and 2 mm (distance-to-agreement) and examined in the global mode without any dose threshold

the method is not sensitive to the part of the energy spectrum below approx. 2 MeV, as such low energy electrons are not effectively transmitted through the beam-forming system of the AQURE accelerator On the other hand, such low energy electrons can only contribute to the PDD at the surface or the most shallow depths where the accurate measurement is challenging as discussed above.

After being implemented into the reconstruction model, the obtained energy spectra were used to simulate PDDs for beams formed by other applicators, i.e., 5 cm and 6 cm diameters. High agreement between the generated and measured PDDs confirms the effectiveness of the proposed method. The discrepancies between the reconstructed and measured distributions concerned, as in the first part of the experiment, the areas near the water surface, i.e. from 0 mm to 3 mm, which, as in the first part, results from measurement inaccuracy in the first layers of the dose build-up area.

Conclusion

The proposed method of solving the inverse Fredholm equation using the Tikhonov regularisation and Dual Annealing method effectively allows the reconstruction of the energy spectra of the electron beams shaped by the applicator with a 10 cm diameter and generated by the AQURE mobile accelerator. These energy spectra can then be successfully used for percentage depth dose reconstruction for different shapes of the electron beam generated by the AQURE mobile accelerator.

Conflicts of interest

Authors declare no conflicts of interest.

Funding

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