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EXPERIMENTAL BENCHMARKING OF SOFTWARE ModeStEB FOR SIMULATION ELECTRON BEAM PROCESSING

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Introduction success of radiation technologies into practice substantially depends on development of computational dosimetry which is based on accurate and validated programs, capable effectively calculate absorbed dose in processes of an irradiation. The simulation of the absorbed dose distributions into thin polyvinylchloride dosimetric films located in the stack of plates of a reference materials irradiated with a scanned electron beam was performed. Modeling of electron beam dose distributions in the multi-layer packages was accomplished using the Monte Carlo method in a three-dimensional geometrical model with utilization of the software ModeStEB. Results of benchmarking experiment for the software ModeStEB, which is used for simulation of industrial electron beam processing, are considered.
KEY WORDS: computational dosimetry, Monte Carlo method, software ModeStEB, dose distribution

ЭКСПЕРИМЕНТАЛЬНАЯ ПРОВЕРКА ПРОГРАММЫ ModeStEB ДЛЯ МОДЕЛИРОВАНИЯ ЭЛЕКТРОННО-ЛУЧЕВЫХ ТЕХНОЛОГИЙ

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Успех внедрения радиационных технологий в практику существенно зависит от развития компьютерной дозиметрии основанной на точных и валидированных программах, способных эффективно рассчитывать поглощенную дозу в процессах облучения. Проведено моделирование распределения поглощенной дозы в тонких поливинилхлоридных дозиметрических пленках, расположенных в пакете пластин из известных материалов, который облучался сканирующим пучком электронов с энергией 10 МэВ. Моделирование распределения поглощенной дозы пучка электронов в многослойном пакете проводилось методом Монте Карло в трехмерной геометрии с использованием программы ModeStEB. Обсуждаются результаты экспериментальной проверки программы ModeStEB, которая используется для моделирования промышленных электронно-лучевых технологий.
КЛЮЧЕВЫЕ СЛОВА: компьютерная дозиметрия, метод Монте Карло, программа ModeStEB, распределение дозы

ЕКСПЕРИМЕНТАЛЬНА ПЕРЕВІРКА ПРОГРАМИ ModeStEB ДЛЯ МОДЕЛЮВАННЯ ЕЛЕКТРОННО-ПРОМЕНЕВИХ ТЕХНОЛОГІЙ

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Успіх впровадження радіаційних технологій у практику суттєво залежить від розвитку комп'ютерної дозиметрії, яка грунтується на точних та валідірованих програмах, здатних моделювати поглинену дозу в процесах опромінення. Проведено моделювання розподілу поглиненої дози в тонких полівінілхлоридних плівках, розташованих у пакеті пластин із відомих матеріалів, які опромінювались скануючим пучком електронів з енергією 10 МеВ. Моделювання розподілу поглиненої дози у багатошаровому пакеті проводилось методом Монте Карло у трьох-вимірній геометрії із використанням програми ModeStEB. Обговорюються результати експериментальної перевірки програми ModeStEB, яка використовується для моделювання промислових електронно-променевих технологій.
КЛЮЧОВІ СЛОВА: комп'ютерна дозиметрія, метод Монте Карло, програма ModeStEB, розподіл дози

Benchmarking (BM) experiment is an integral part of validation of each software for simulation of radiation processing. There are many examples of BM experiments for various types of software for simulation of industrial radiation processing [1-7]. Main part of these BM experiments are based on comparison of simulation and measurement results for an absorbed dose distributions in targets with specific geometry irradiated with electron beam (EB), X-ray and gamma ray on specific radiation facility. This complicates performing of BM for other software developers.

Authors approach for BM experiments is based on investigations, where each BM experiment for developed software was sensitive to features or physical regularities of absorbed dose distribution formation in an irradiated target

[4-7]. For example, such types of features and physical regularities for electron absorbed dose were observed at investigations of boundary effects with a high dose gradient which appear near the interface of contacting materials with different density and/or atomic number irradiated in parallel with EB [4-7].

The objective of this study was the performing of BM experiment which includes verification of theoretical prediction for EB dose distribution formation in a stack of plates interleaved with PVC (polyvinylchloride) dosimetric films (DFs). Such type of stacks are used in radiation processing dosimetry. To validate the ModeStEB software, point-by-point comparisons was made between theoretical predictions and dosimetric results.

GEOMETRICAL AND SIMULATION MODELS OF EB FACILITY AND IRRADIATED PRODUCT

Schematic representation of the EB facility used for simulation of the electron depth dose distributions in the stack with dosimetric films irradiated with scanned EB and on moving conveyor is shown in Fig. 1.

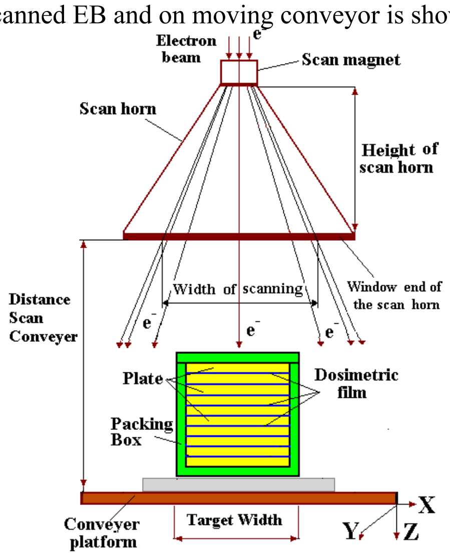


Fig. 1. Electron beam and irradiated dosimetric stack geometry.

Arrangement of a stack plates interleaved with dosimetric films on moving conveyor irradiated with triangular scanned EB. The stack with dosimetric films located in closed packing box. Axis Z - direction of EB incidence, axis X - direction of EB scanning, axis Y - direction of conveyer motion.

Dosimetric stack consists of a set of plates made of an arbitrary materials interleaved with dosimetric films or a stack of dosimetric films alone. The number of plates with dosimetric films in the stack is in the range from 1 to 60. The plates of stack with dosimetric films can be located on the conveyer platform perpendicular or parallel relatively incident EB axis. The stack with dosimetric films can be located in open or closed packing box.

Simulation of EB dose distributions in an irradiated films located in the stack was accomplished the with the Monte Carlo (MC) method in a tree-dimensional (3-D) geometrical model by the programs ModeStEB. In accordance with the schematic representation of electron beam facility and multi-layer target presented in Fig. 1 a source of electron beam including spectral characteristics, a scanner, a conveyor line and an irradiated target are considered as uniform self-consistent geometrical and physical models.

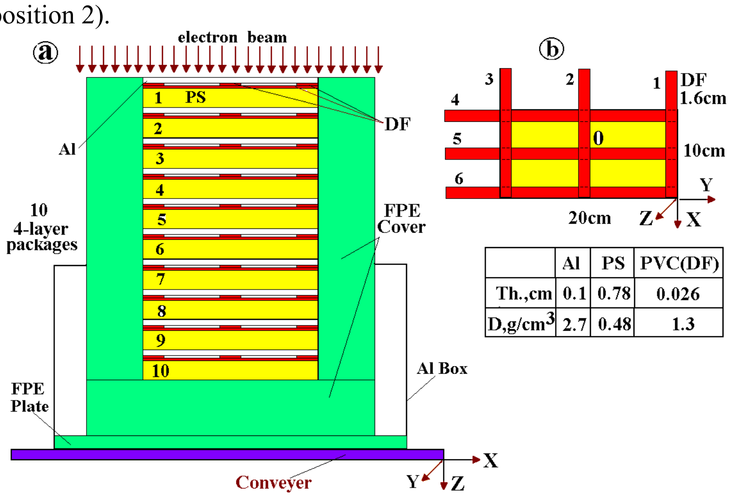
The following processes of interaction of electrons with substance and their modeling conceptions were included in the physical model of software ModeStEB: electrons lost energy by two basic processes an inelastic collision with atomic electrons and bremsstrahlung; inelastic electron collision with atomic electrons lead to excitation and ionization of the atoms along the path of the particles (model of grouping of the transferred energy); emission of the secondary electrons (model of the threshold energy); electrons participated in elastic collisions with atomic nuclear lead to changes in the electron direction (model of grouping of transferred pulse).

In the default mode of the software ModeStEB, the values of energy cut off and threshold energy of electrons are selected in automatic regimes to provide the necessary space distribution for absorbed dose of electrons in thin film. All physical processes which assure obtaining of results with predetermined accuracy are taken into account at simulation of an absorbed dose distribution of electrons. For example, for EB radiation processing in the energy range of incident electrons from 100 keV to 10 MeV and irradiated materials with atomic number $Z \leq 30$, the model uncertainty is less than 5% for calculated dose distribution in the field of the basic EB energy absorption.

BM experiment includes verification of theoretical prediction for EB dose distribution formation in a stack of plates interleaved with PVC dosimetric films. The stack consists of 10 packages. Each package includes 4 layers: 1st layer -Aluminum plate with thickness 0.1cm and size 20x10cm (density 2.7 g/cm^3), 2nd and 3d layers - PVC film in form of strips with thickness 0.026 cm, 1.6cm – width, 10cm and 20 cm length (density 1.3 g/cm^3), and polystyrene (PS) plate with thickness 0.78cm and size 20x10cm (density 0.48 g/cm^3). The stack was inserted in the open Ethafoam box with density of 0.1 g/cm^3 and wall thickness 5 cm from all sides of the stack. Stack size of all plates with dosimetric films along EB axis (7.12 g/cm^2) was greater than electron range with energy 9.7 MeV.

Setup for a multi-layer target in the form of stack of plates with dosimetric films on a conveyer platform are shown in Figs. 2(a) and (b). The stack of plates with dosimetric films was placed on a foam plate (thickness of 5 cm) in the center of a standard aluminum box (580x460x200 mm) and a wall thickness of 1 mm. The aluminum box with the stack of plates with dosimetric films was placed into the central line of the conveyer platform.

Two series BM experiments were performed. In the 1st series irradiation, the stack was located on a conveyer platform in a such way that side of plates in the stack with size 20cm was oriented in direction of EB scanning (See Fig.3, position 1). In the 2nd series irradiation – side of plates in the stack with size 10cm was oriented in direction of EB scanning (See Fig.3, position 2).



	Al	PS	PVC(DF)
Th.,cm	0.1	0.78	0.026
D,g/cm^3	2.7	0.48	1.3

Fig. 2. (a) Arrangement of a stack of plates with dosimetric films in form of strips on moving conveyor irradiated with triangular scanned EB. Surface of plates is located transversely to EB axis. The stack consists of 10 identical 4-layer packages.
(b) Location of PVC dosimetric films in the 2nd and 3d layers. 3 DFs with 10 cm length are located in 2nd layer, number 1, 2, 3. 1 DF (number 1) is located on the center of 20 cm plates, and 2 DFs (number 1 and 3) are located on the boundary of 20 cm plates with Ethafoam box (FPE). 3 DFs with 20 cm length are located in 3d layer, number 4, 5, 6. 1 DF (number 5) is located on the center of 10 cm plates, and 2 DFs (number 4 and 6) are located in the boundary of 10cm plates with foam polyethylene box. The DFs with 10 cm length are transversely placed above the DFs with 20cm length. Center intercrossing of strips with length 20cm and 10 cm is marked by point 0.

Proposed simulation and experimental models of the stacks of plates with dosimetric films allows completely to restore the EB dose map in multilayer target and to make a correct analysis for EB dose field formation in the dosimetric films located between plates of the stack.

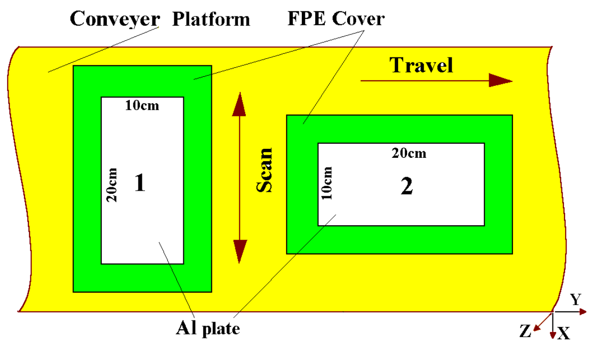


Fig. 3. Top view of two arrangements of a stack of plates with dosimetric films on moving conveyor.
Position 1 - side of plates in the stack with size 20cm is oriented in direction of EB scanning.
Position 2 - side of plates in the stack with size 10cm is oriented in direction of EB scanning.

MATHEMATICAL MODELING OF EB DOSE DISTRIBUTION IN STACK OF PLATES WITH THIN FILMS

Software ModeStEB was used for investigation and analysis of EB dose distribution formation in the thin films located between plates of the stack which is presented in Fig.2 [8]. In simulation model the stack was located on moving conveyer in two positions in accordance with Fig.3 and irradiated by scanned EB with energy 9.7 MeV. 2-D and 3-D dose distributions of 9.7 MeV electrons in the PVC films were simulated with MC methods for each films located in the 2nd and 3d layers from 1st to 10th packages. 2-D dose distributions were calculated in the center of plates and near the interface of stack plates with FPE cover. The EB dose distribution in the irradiated DFs located in the stack is represented as a function of two coordinates: the scan direction (axis X), and the conveyer motion (axis Y). The dose value in PVC DF was averaged along film thickness (axis Z). At visualization of results simulation of 3-D dose distributions in DF, the bin size is 1/20 of the film width in direction of EB scanning (axis X) and 1/20 of the film length in direction of conveyer motion (axis Y).

Modeling of EB transport from the exit window of accelerator to the incident surface of the irradiated target takes into account such effect as scattering of electrons in an air gap. Computer modeling was chosen so that in the selected range of absorbed doses the relative root-mean-square statistical error was less than 1%.

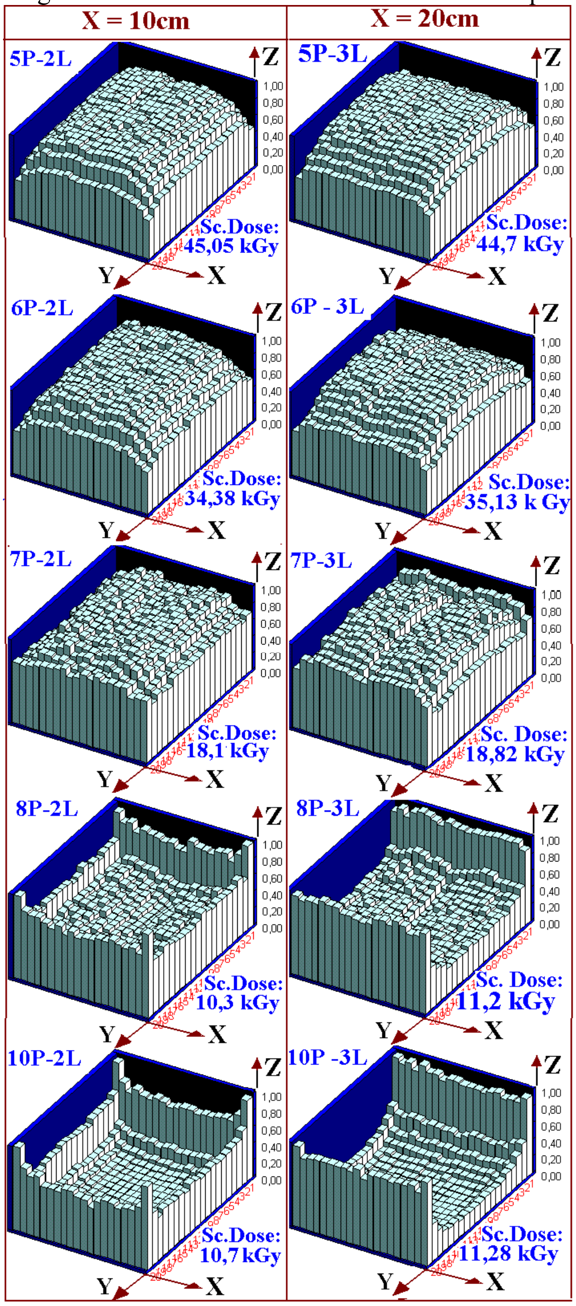


Fig.4. Results of MC simulation of 3-D dose distributions of 9.7 MeV electrons in the PVC films located between plates of the stack. Sc.Dose - scaling Dose.
Row X=10cm, PVC films with length 10cm located between plates of the stack along scan direction for the 5th, 6th, 7th, 8th and 10th packages, respectively. Stack located on conveyer platform in accordance with position 2 in the Fig.3. Row X=20cm, PVC films with length 20cm located between plates of the stack along scan direction for the 5th, 6th, 7th, 8th and 10th packages, respectively. Stack located on conveyer platform in accordance with position 1 in the Fig.3.

The results of MC simulation of 3-D dose distributions of 9.7 MeV electrons in the PVC films with length 10cm (row X=10cm) and 20cm (row X=20cm) located in the 2nd and 3d layers respectively along scan direction for the 5th, 6th, 7th, 8th and 10th packages are shown in Fig.4.

The form differences of EB absorbed dose map in the PVC films from 5th to 10th packages for each stack positions 1 and 2 on a conveyer platform are observed in the Fig.4. The form differences of EB absorbed dose distribution in the PVC films for the 8th and 10th packages are observed between stack positions 1 and 2 on a conveyer platform.

Analysis of simulation results for the EB absorbed dose field formation in the multi-layer structure of the stack irradiated with the scanned EB with energy 9.7 MeV on a moving conveyer have shown the following features:

• Starting with 2nd package, the value of absorbed dose in the PVC dosimetric films near the interface of package with Ethafoam packing box is reduced about in 10-40 percent on the length from interface up to 4 cm in comparison with the package center. D_{max} - dose maximum is located in the center of PVC DF (center stack). D_{min} - dose minimum is located near the interface of PVC DF with Ethafoam cover.

This effect is explained by the balance disruption of primary and secondary electrons near the interface of stack plates with Ethafoam cover.

• Starting with 5th package, there are “shadow” in the absorbed dose distribution for PVC strips with 20 cm length from 10cm PVC strips, which were placed above 20 cm PVC strips and crossed each other in the center of plate plane (See point 0 in the Fig. 2 (b)).

• For the 9th, and 10th packages, the values of the EB absorbed dose in the center of the PVC DF plates tends to 0 with increasing a layer number. Such tendency is observed because of thickness of all stack plates with dosimetric films in 9 and 10 packages along EB axis is greater than EB range with energy 9.7 MeV.

• Beginning with the 8th PVC DF layer, an appearance of the local maximum for the dose distribution near the interface of DF with an Ethafoam cover is observed near all packages sides - from sides located in direction of EB scanning and in direction of conveyer travel. D_{max} for these layers is located near the interface of PVC DF with Ethafoam cover. D_{min} is located in the center of PVC DF (center stack).

An appearance of the local maximum can be explained by the lateral highlighting with the flux of primary and secondary electrons released from Ethafoam cover into DF. The reason is that the range of 9.7 MeV electrons in the Ethafoam cover is greater than range of electrons in the stack materials.

• The local maximum for the EB dose distribution near the interface of DF with Ethafoam cover in the 9th and 10th packages is observed on the depth (along axis Z) greater than the EB range in the stack materials.

• The values of local maximums for the EB dose distribution near the interface of DFs with an Ethafoam cover in the strips with length 20 cm and in the length 10 cm in the 8th, 9th and 10th packages are essentially depended on their orientation on the conveyer platform – ether in the direction of

EB scanning or in the direction of conveyer travel.

• The ratios of local maximums in the EB dose distributions in the strips with length 20 cm are approximately 2.5, and in the strips with length 10 cm approximately 1.5 times for the 8th, 9th and 10th packages; this is greater for strips located in direction of conveyer travel in comparison with strips located in direction of EB scanning.

• The value of local maximum for the EB dose distribution near the interface of DF with the Ethafoam cover in the strips with length 20 cm in the 8th, 9th and 10th packages in direction of EB scanning is less than about half the value of the local maximum in the strips with length 10 cm for the same packages.

• The values of local maximums for the EB dose distribution near the interface of DFs with the Ethafoam cover in direction of conveyer travel are approximately equal for dosimetric strips with length 10cm and 20cm.

• The specific 3-D boundary effects are observed in the area of the stack's corners. These effects are appeared in the corners due to summation of boundary anomalies in direction of conveyer travel and in direction of EB scanning.

Experiments were performed for confirmation of MC predictions for EB dose distributions in the thin films located between plates of the stack irradiated with scanned EB on the moving conveyer in accordance with geometrical model presented in Fig.2.

RESULTS AND DISCUSSIONS

Irradiation of multi-layer target in the form of stack of plates with dosimetric films was performed on the electron linear accelerator Elektronika 10/10 at INCT, Warsaw with electron beam energy of 10 MeV [9].

The stack was irradiated with a scanned electron beam of energy 9.7 MeV, pulse duration 5.6 µs, pulse frequency 370 Hz, average beam current 1.04 mA, scan width 58 cm, conveyer speed was in the range 1-0.1 m/min, scan frequency 5 Hz, angular spread 6 degree. Electron beam energy was measured with standard Al wedge. Control of dose delivered to the target in time irradiation was performed with RISO polystyrene calorimeters [10].

The absorbed dose of irradiated materials was delivered in the range of 5-80 kGy. The maximum of combined uncertainty related to dose determination in the heterogeneous target with the PVC dosimetric film for values of doses greater than 5 kGy did not exceed 8% (k=2). The uncertainty is a combination of the uncertainties related with dosimetric film calibration, in reproducibility of the series of experiments, the dose given at electron accelerator, spectrophotometer reader variability. The uncertainty of the length value measurement of dosimetric strips is 0.1cm.

PVC dosimetric film was calibrated against alanine dosimeter which is traceable to National Physical Laboratory, Teddington, Middlesex, UK [www.npl.co.uk]. A SEMCO S/E_c spectrophotometer in automatic regimes was used for reading optical density at a wavelength of 394 nm from PVC strip films with a step of 0.1 cm along the film length.

In two series BM experiments the stack was irradiated twice (See Fig.3, Positions 1 and 2). In the first irradiation, an absorbed dose was delivered to the PVC strips located in the 2nd an 3d layers along scan direction in the 1st, 2nd, 3d, 4th, 5th, 6th and 7th packages in the range of 5-80 kGy. In the second, an absorbed dose was delivered to the PVC strips located in the 2nd an 3d layers along scan direction in the 7th, 8th, 9th and 10th packages in the range of 5-80 kGy. Normalization of all curves of absorbed dose distribution along scan direction from the 1st up to 10th package in each series was performed on the maximal value of an absorbed dose in the PVC dosimetric films located in the 2nd and 3d layers of the 7th package.

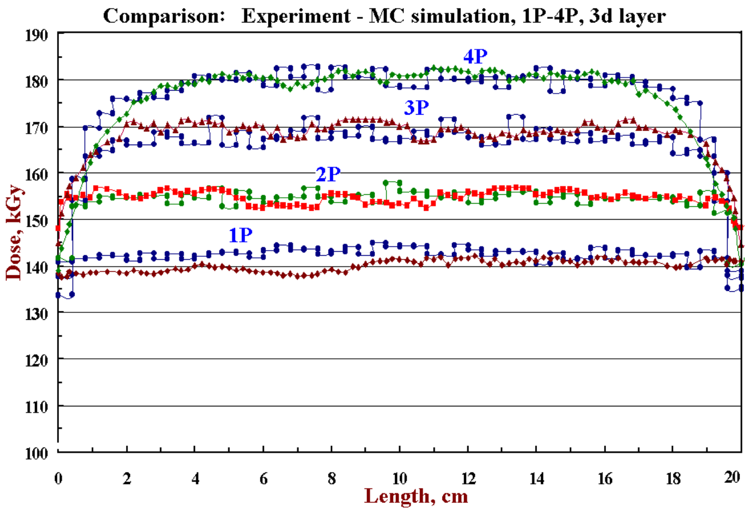


Fig.5. Absorbed dose distribution in PVC strips with length 20cm located in the 3d layers along scan direction for the 1st, 2nd, 3d, and 4th packages, respectively. Round points – results of MC simulation.

A comparison of the results from the MC simulations and experimental measurements of dose distributions of 9.7 MeV electrons in the PVC films with length 20cm located in the 3d layers along scan direction for the 1st, 2nd, 3d, and 4th packages is shown in Fig.5. PVC strip is located in the center of the plate along travel direction; see position position 5 in the Fig. 2 (b). The bin size of the 2D-view of dose distributions is 1/50 of the film length (axis X). The uncertainty of the length value of all curves for dosimetric strips is 0.1cm and the average size in each point is 0.1cm.

As is seen from Fig.5, beginning with 2nd package, the value of absorbed dose in the PVC dosimetric films near the interface of package with Ethafoam packing box is reduced by about 10-40 percent over the distance from the interface to 4 cm inwards, in comparison with dose recorded at the package center.

A comparison results from MC simulations and experimental measurements of dose distributions of 9.7 MeV electrons in the PVC films located in the 3^{d} layers along scan direction for the 5th, 6th, 7th, 8th, 9th and 10th packages is shown in Fig.6. PVC strip is located in the center of plate along travel direction, see position 5 in the Fig. 2 (b).

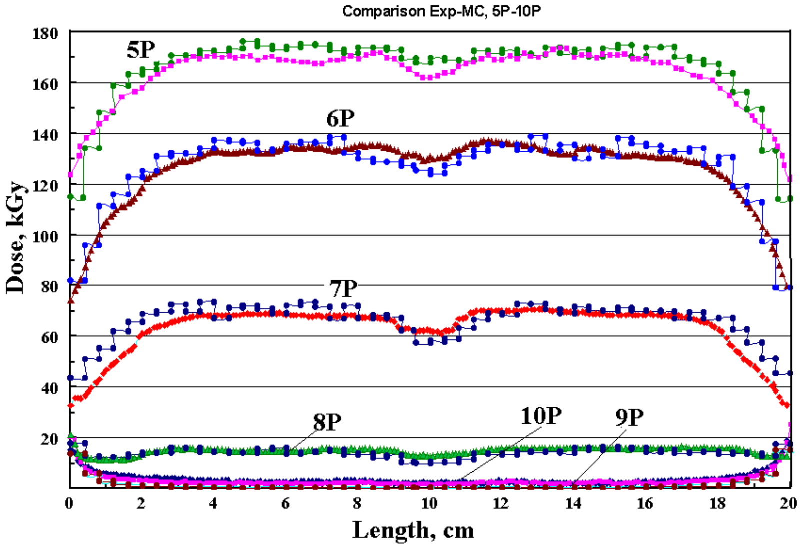


Fig.6. Absorbed dose distribution in PVC strips with length 20cm located in the 3^{d} layers along scan direction for the 5th, 6th, 7th, 8th, 9th and 10th packages, respectively. Round points – results of MC simulation.

As is seen from Fig.6, beginning with the 5th package, there are “shadows” in the absorbed dose distribution for PVC strips with 20 cm length from 10cm PVC strips, which were placed above 20 cm PVC strips and crossed each other in the center of plate plane. For the 8th, 9th and 10th packages, the values of the EB absorbed dose in the center of the PVC DF plates tends to 0 with increasing of a layer number. For the 8th, 9th and 10th packages, an appearance of the local maximum for the dose distribution near the interface of DF with Ethafoam cover in direction of EB scanning is observed.

A comparison of the results of MC simulation of 3-D dose distributions of 9.7 MeV electrons in the PVC films with length 20cm located in the 3^{d} layer along scan direction for the 5th, 6th, 7th, 8th and 10th packages is shown in Fig.4. (Row X=20cm).

A comparison of the results of MC simulation and experimental measurements of dose distributions of 9.7 MeV electrons in the PVC films with length 10cm located in the 2nd layer along scan direction for the 6th, 7th, 8th, 9th and 10th packages is shown in Fig.7. PVC strip are located in the center of the plate along the travel direction, as shown in position 2 in the Fig.2 (b).

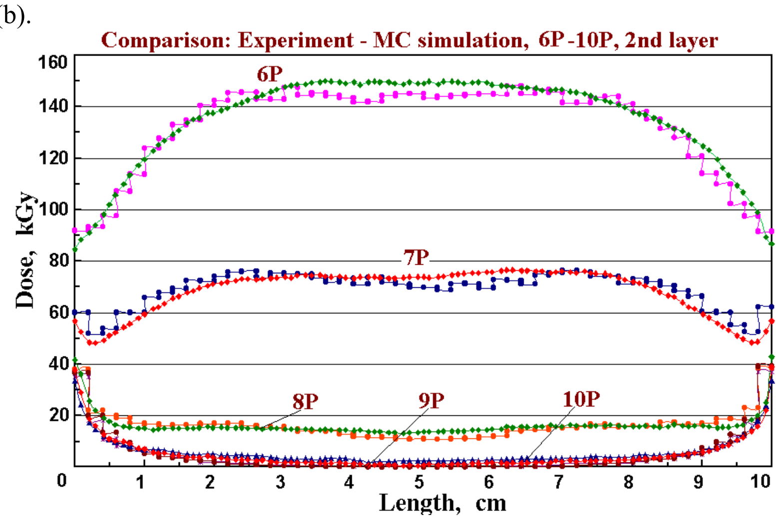


Fig.7. Absorbed dose distribution in PVC strips with length 10cm located in the 2nd layers along scan direction for the 6th, 7th, 8th, 9th and 10th packages, respectively. Round points – results of MC simulation.

As may be seen from Fig.7 for the 8th, 9th and 10th packages, an appearance of the local maximum for the dose distribution near the interface of DF with an Ethafoam cover in direction of EB scanning is observed. The value of local maximum for the EB dose distribution near the interface of DF with an Ethafoam cover in the strips with length 10 cm in the 8th, 9th and 10th packages in direction of EB scanning is more than twice the value of local maximum in the strips with length 20 cm for the same packages. For the 8th, 9th and 10th packages, the values of the EB absorbed dose in the center of the PVC DF plates approaches 0 with increasing layer number.

CONCLUSION

The measurement results of the absorbed dose distribution of 9.7 MeV electrons in the PVC film are in agreement by the shape and absolute value with the results obtained on the basis of the simulation of an irradiation process using the MC method with software ModeStEB.

The boundary anomalies with a high dose gradients for an absorbed dose near the interface of contacting plates with different densities and/or atomic number and near the interface of plates with packing box were observed. It was established theoretically and experimentally that maximum for the EB dose distribution near the interface of DF with a wall of the Ethafoam box is observed on the depth greater than the electrons range in the stack materials. An appearance of the maximum for EB dose distribution can be explained by the lateral highlighting with the flux of primary and secondary electrons released from Ethafoam cover into DF. Such effect is one of an important mechanisms of dose distribution formation in three-dimensional objects irradiated with EB.

Theoretical and experimental observations of such physical regularities can be a good examination of software for simulation EB processing. The software ModeStEB can be used as research tools for investigations of the features and physical regularities for an EB dose distribution formation in multi-layer targets. In practice the software ModeStEB can be used: for dose mapping studies to identify the zones with maximum and minimum doses in an irradiated product; as computational dosimetric device for determination an energy of incident electrons, an EB ranges, prediction and analysis of the EB absorbed dose characteristics related with parameters of EB radiation facility, as well as an interpretation of experimental dosimetry results. The software can be used also to optimize the design for new EB irradiator, for commissioning of EB facility, EB facility qualification, process validation and routine process control.

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