DEVELOPMENT AND VALIDATION OF SOFTWARE FOR SIMULATION OF PRODUCT PROCESSING REGIMES AT AN ELECTRON ACCELERATOR

V.I. Nikiforov, N.M. Pelichatyi[1], R.I. Pomatsalyuk, Yu.V. Rogov, V.A. Shevchenko, A.Eh. Tenishev, V.L. Uvarov

National Science Center "Kharkov Institute of Physics and Technology", Kharkov, Ukraine;
[1]V.N. Karazin Kharkov National University, Kharkov, Ukraine
E-mail: uvarov@kipt.kharkov.ua

On the basis of the PENELOPE-2008 transport code, the three fundamental SW complexes for the modelling of processes in objects of various geometry and materials exposed to the scanned electron beam have been developed. For testing, the electron range and stopping power as well as photon absorption coefficients for different materials in the particle energy range 1…30 MeV were calculated. The results obtained were compared with the reference data given in the ICRU Report 35. At the second stage of validation, the computation and measurement of the absorbed dose in the standard polystyrene calorimeter as well as the dose distribution in the rectangular phantom passing via the zone of exposure to the scanned electron beam were conducted. Application of the developed SW enables the analysis and optimization of the industrial irradiation regimes.

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INTRODUCTION

Recently, active development of techniques for computer modelling of processes of the ionising radiation (mainly, accelerated electrons, X-ray and gamma radiation) interaction with the substance is observed. It is caused by constant expansion of spheres and volumes of radiation application in industry, medicine and other areas, and also by the increase of requirements to quality of radiation technology implementation [1]. The basic demand is keeping the absorbed dose of radiation, D, in any point of the processed product in the range

$$D_{min} \leq D \leq D_{max}, \quad (1)$$

where D_{min} and D_{max} are the minimum and maximum values of the dose imposed by technological regulations, respectively. For example, in case of radiation sterilisation, D_{min} corresponds to the value of the sterilization dose [2].

Ensuring the condition (1) execution by means of the direct measurement of the dose distribution within each item is practically impossible considering a bulk of the processed product (usually, thousands cubic metres). The standard decision of the problem is the keeping of key parameters of the process in specified ranges governing the dose distribution in the given object, while a direct dose control in specified points of selected objects.

In case of the technological installation with the electron accelerator such parameters are [2]:

- electron energy;
- average beam current;
- width and shape of the beam scan;
- conveyor speed.

Corresponding SW based on these data enables to calculate dose distribution within all volume of the irradiated object, and also, that is not less important, to pick up the optimum regime of the processing for each kind of the product, satisfying to the condition (1) at the minimum expense of the radiation resource.

By now, it has been developed a number of transport codes on the basis of the Monte Carlo method, allowing the modelling of processes of radiation interaction with substance (Geant, PENELOPE, MCNP, FLUKA, EGS4, etc.). As a result of the analysis of references as well as of own preliminary study data on the accuracy of simulation of the electron-photon cascade transport in the substance, a program system PENELOPE [3] has been chosen as the basis. This package is intended for the decision of stationary problems and cannot be directly used for the dose calculation in objects moved through the zone of irradiation with the scanning beam.

The communication deals with results of updating of the PENELOPE-2008 code, and also of validation of the SW developed in such a way on its compliance with demands set by governing bodies on radiation technology processes.

1. SW STRUCTURE

The main objective of the modelling is an ascertainment of the state of radiation and its absorbed energy (dose) for the object in whole or for its separate part. To solve this problem, an algorithm of the basic PENELOPE package was modified (see the scheme in Fig. 1, added operators and references to new program modules are framed). In particular, the package has been added with the three program complexes providing a consecutive description of primary radiation, its transport to the irradiated object and the interaction with it.

So a program complex "BEAM" provides a description of the electron beam at the exit of the accelerator. Modules of the complex model the random values of energy and co-ordinates of points of the electron escape within the beam cross-section with the set distribution of the probability density

Modules of the "TRANSPORT" complex together with modules of "BEAM" are intended for the simulation of processes of the electron, photon and positron transport in the various media, and also for the registration of the probability density distribution of the particle state relative to the energy, radius and angle in various points of modelled installations and objects.

A complex "DOSE" is intended for the modelling and optimisation of the product processing regime at the accelerator with the scanned electron beam relative to the absorbed dose distribution.

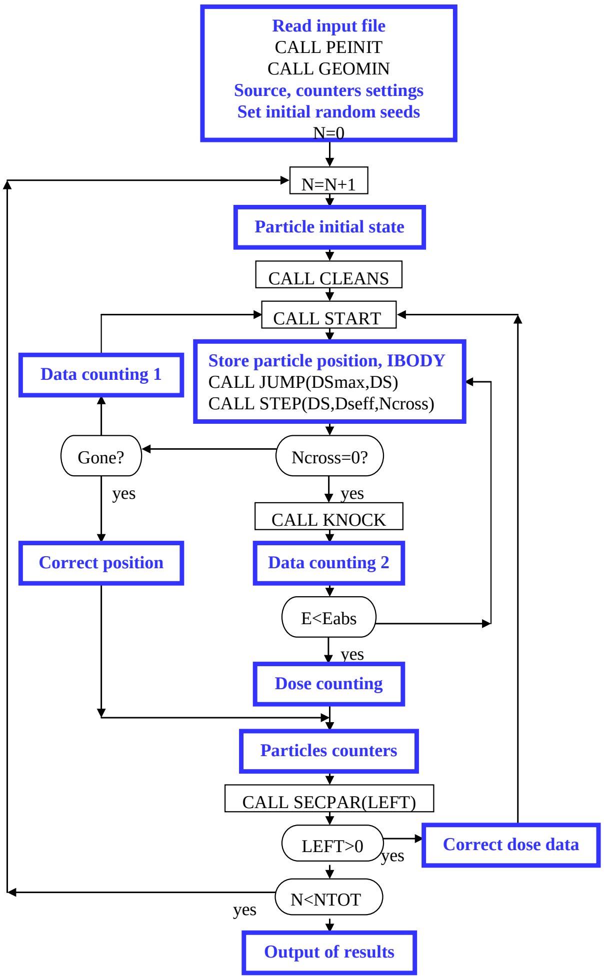

Fig. 1. Scheme of modified algorithm of PENELOPE main program

In case when the modelling of radiation processes in the concrete installation is needed, a special main program is developed as well as a file with its initial parameters, a corresponding readout module, a file with the description of the simulated system geometry, and also a file of materials. For readout of radiation characteristics in various points as well as of results of the radiation influence on the irradiated object, special soft modules- transducers were brought into service.

2. SW VALIDATION

2.1. COMPARISON WITH REFERENCE DATA

2.1.1. Testing of the developed package was conducted in the two stages. At the first stage, a study of the adequacy of the modelling of basic radiation processes has been executed, beginning from the description of the primary electron beam and finishing with the determination of principal characteristics of its interaction with material media. As an example, some results of the complex "BEAM" application for the description of beam profile and spectrum of the accelerator KUT-30 [4] are shown in Fig. 2.

2.1.2. For testing of the complex "TRANSPORT", dependences of the range (Fig. 3,a) and stopping power (Fig. 3,b) on electron energy as well as of the photon mass attenuation coefficient on their energy (Fig. 4) in various materials were calculated.

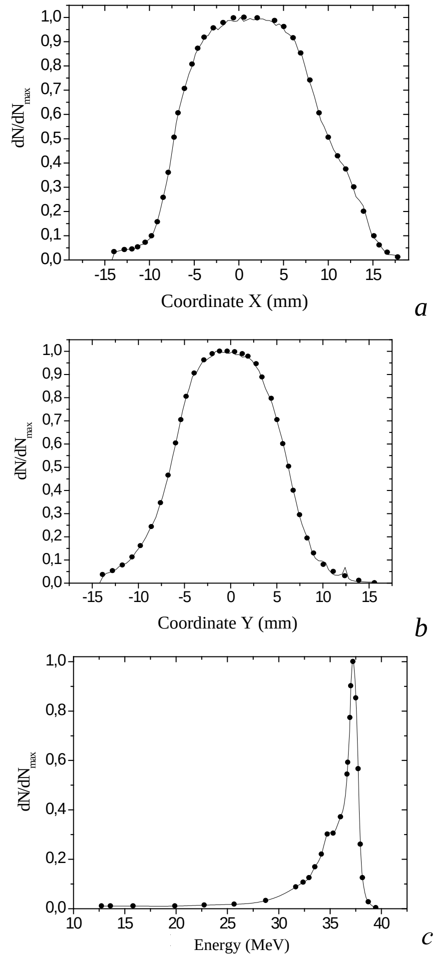

Fig. 2. Comparison of normalized experimental (dots) and simulated (solid curves) electron distributions (a, b) and beam spectrum (c)

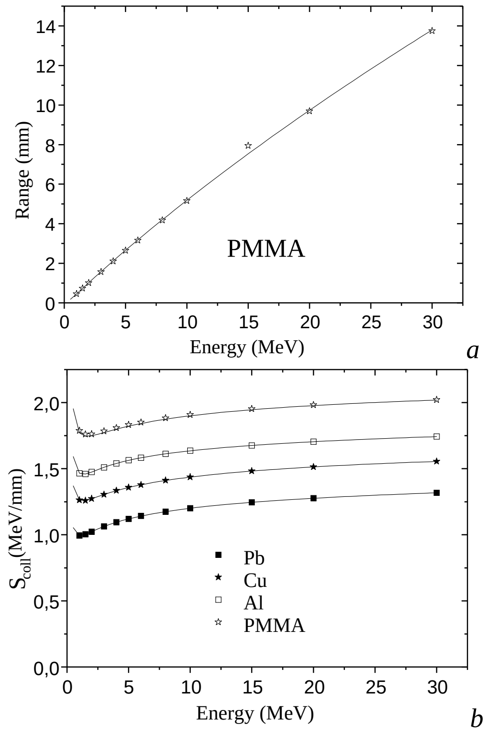

Fig. 3. Range in PMMA (a) and stopping power of electrons in a number of materials (b): solid curves - calculation, dots - data from the work [5]

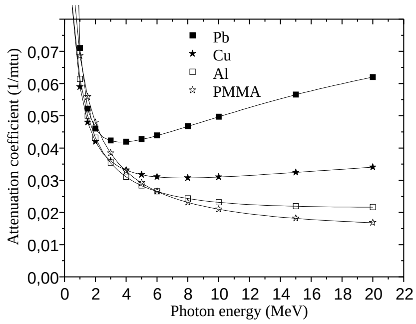

Fig. 4. Dependence of photon attenuation coefficient on their energy: solid curves - calculation, dots – data from the work [6]

2.1.3. For the purpose of the complex "DOSE" examination, the distribution of the absorbed energy of the electron beam at different electron energy in a number of materials was calculated (Fig. 5).

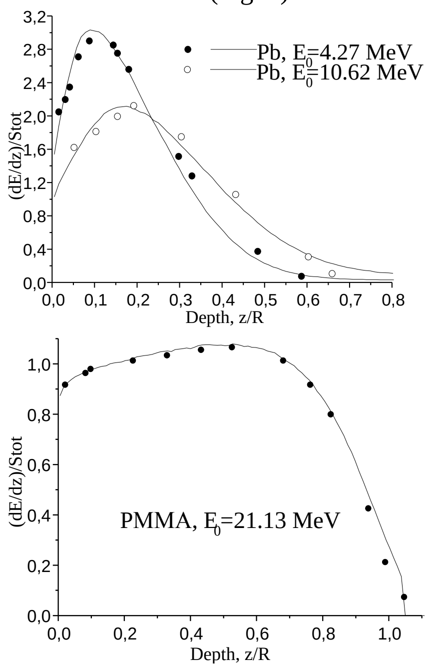

Fig. 5. Absorbed energy as function of normalized depth in various materials at their irradiation with electrons: z-depth, R-electron range in continuous slowing-down approximation, S_{tot}-total mass stopping power of material. Solid curves-result of simulation, dots- data from the work [5]

2.2. BENCHMARK EXPERIMENTS

2.2.1. A power supply of the beam scanner of the LU-10 Linac is controlled by PC [7]. It provides a possibility for the operator to set any shape of the beam sweep. In particular, at carrying out of testing experiments it was sinusoidal for the one half-cycle and linear for the other (Fig. 6). Such mode of the scanning allows to decrease the factor of non-uniformity of the dose distribution, D_{max}/D_{min}. The dependence of the beam deviation angle on time was defined by conditions

$$\theta = \begin{cases} F_1\left(t - kt_0\right), at\ (k-0.25)t_0 < t < (k+0.25)t_0, \\ F_2\left(t-(k+0.5)t_0\right), at\ (k+0.25)t_0 < t < (k+0.75)t_0, \end{cases} \qquad (2)$$

where k=0,1,2… is the number of the beam scanning period.

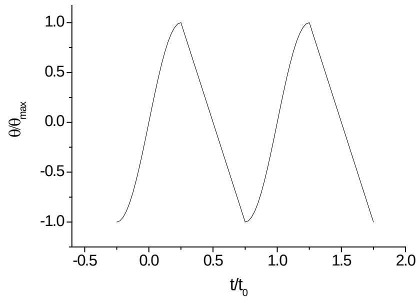

Fig. 6. Shape of beam sweep at benchmark experiments (θ_{max} – amplitude of beam deviation angle; t_0 – period of scanning)

In the course of the modelling, as random quantities the position of the irradiated object relative to the plane of the beam scanning (Fig. 7) and also, the interaction of accelerated electrons with the object were considered taking into account cyclic boundary conditions (2).

The calculated value of the dose, D_c, was determined from the expression

$$D_c = \frac{I \cdot H}{V \cdot N}\sum_{i=1}^{N} D_i\ , \qquad (3)$$

where *H* is the conveyor period (the distance between equivalent surfaces of neighbour objects), *V* is the conveyor speed, *I* is the beam current, D_i is the dose in the point with co-ordinate x_i, *N* is the number of events.

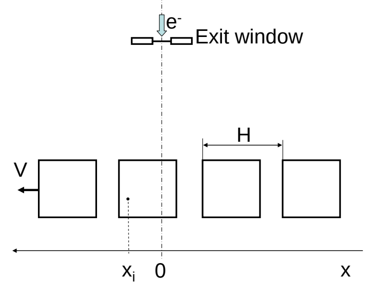

Fig. 7. Scheme of modelling of moving object irradiation with scanning electron beam

2.2.2. For the estimation of adequacy of calculation of the absorbed dose in the moving object under influence of the scanned electron beam, a standard polystyrene calorimeter, commonly applied as a reference dosimeter of electron radiation [8], was used as such object. It represents a parallelepiped from cellular polystyrene measuring 29×29×10 cm, in the centre of which a body of the calorimeter in the form of the disk from polystyrene of 138 mm diameter and 18 mm thick is situated. In the disk, there a thermistor is inserted with contacts leading to the external surface of the calorimeter.

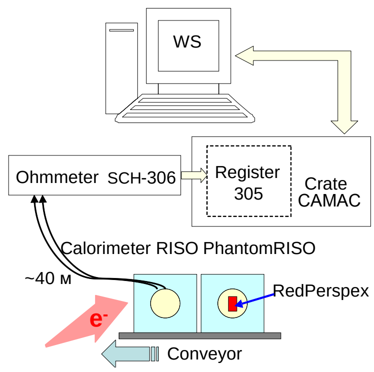

Fig. 8. Scheme of absorbed dose on-line measurement

The absorbed dose is determined on the change of the calorimeter body temperature as a result of irradiation, measured from the thermistor resistance. The scheme of the measurement is represented in Fig. 8.

The polystyrene calorimeter RISO and phantom RISO, completely identical to the calorimeter, were positioned on the transport container of the conveyor of irradiation installation with the accelerator LU-10 [9]. In the phantom, routine dosimeters of the Red Perspex 4034 type [10] were placed. The transport container together with calorimeter and phantom were passed with specified velocity through the zone of irradiation. In the on-line mode, the measurement of the calorimeter resistance via a two-wire line with the use of the ohm-meter SCH-306 was made. The digitized values of the calorimeter resistance were read out in the module of the register 305 located in the crate CAMAC and processed in the operator workstation WS. Interval of the information read out was set by operator and made 2 seconds. The data on thermistor resistance before-, during- and after irradiation were unloaded in the graphic form and downloaded in the file. As a result of their following processing in accordance with the procedure [8], the value of the calorimeter temperature, and also of the absorbed dose in it and in the phantom was determined (Fig. 9). In the course of measurements, the average electron energy made 9.6 MeV, the beam current 780 μA, the width of the sweep at the front plane of calorimeter and phantom was 44 cm.

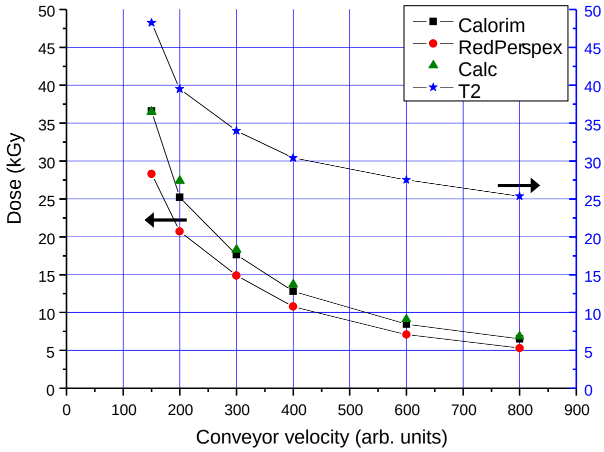

Fig. 9. Results of measurement of calorimeter temperature and absorbed dose

Analysis of data in Fig. 9 shows, that values of the dose calculated and measured using the calorimeter technique differs generally no more than on 5%. It is in agreement with the value of the error of measurements provided with the calorimeter. The observed systematic underestimating of the dose, measured with the Red Perspex dosimeters, can be explained by their calibration on the gamma source. In case of electron radiation, a dose rate is by ~ three order of values higher. Therefore, as a result of the detector heating by radiation its sensitivity decreases [10].

2.2.3. Next series of testing experiments was conducted with the use of the specially designed 3D-phantom (Fig. 10). It corresponds a parallelepiped from cellular polystyrene with density 0.114 g/cm^3 measuring 79×37×39 cm. The phantom contains a net of slots for placing Red Perspex dosimeters. Devices of such type are recommended for dose mapping at certification of facilities for radiation processing [2].

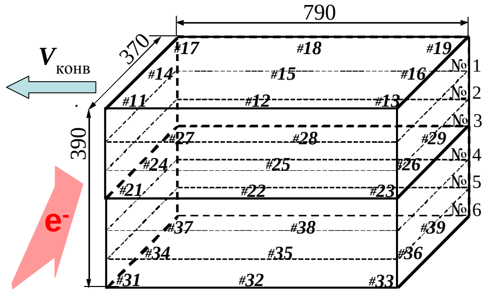

Fig. 10. 3D-polystyrene phantom

Using the developed SW, the calculation of the dose distribution in the phantom for the irradiation regime realised in the experiment was executed. The beam current made 800 μA, the electron energy – 9.6 MeV. The phantom moved through the irradiation zone at a velocity of 1.2 cm/sec. Results of the measurement and calculation of the dose distribution along the central axis of the phantom as well as data of the analysis of inhomogeneity of the dose distribution in the phantom at its two-sided irradiation are summarized in Fig. 11 and in the Table. Results of the Red Perspex dosimeter calibration by means of the RISO calorimeter technique (see Fig. 9) were used at the dose measurement. The difference between calculated and experimental data can be explained by the accuracy of the dosimeter calibration, instability of beam parameters, and also by rolling oscillations of the transport container with the phantom at its passage through the irradiation zone.

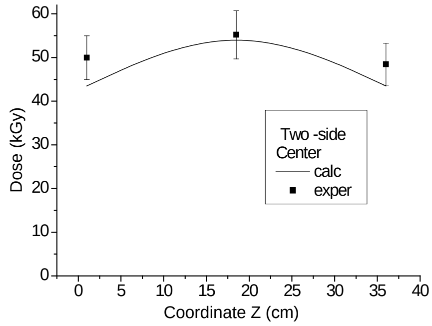

Fig. 11. Dose distribution along central axis of phantom

Characteristics of dose field inhomogeneity in the phantom (two-sided irradiation)

	Experiment	Calculation
№ of point with D_{max}	25	25
№ of point with D_{min}	13	13
D_{max}/D_{min}	2.47	2.21

CONCLUSIONS

The software has been developed and tested for the modelling of processes of influence of the scanned electron beam with any shape of the sweep on objects moving at any velocity through the irradiation zone.

At designing of main programs for the modelling of particle transport, a special attention was paid to the control of the balance of their quantity and energy in the system in whole, and also to the calculation of basic characteristics of particles, which are absorbed in the system and left it. The designing of main programs has been executed in such a way, that the calculation of listed characteristics does not depend on the degree of complexity of the simulated installation.

SW provides a possibility of calculation of the absorbed dose and its distribution within irradiated items, as well as optimisation of irradiation modes, and also estimation of the accuracy of dosimetry system calibration in the field of electron radiation.

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РАЗРАБОТКА И ВАЛИДАЦИЯ ПРОГРАММНОГО ОБЕСПЕЧЕНИЯ ДЛЯ МОДЕЛИРОВАНИЯ РЕЖИМОВ ОБРАБОТКИ ПРОДУКЦИИ НА УСКОРИТЕЛЕ ЭЛЕКТРОНОВ

В.И. Никифоров, Н.М. Пелихатый, Р.И. Помацалюк, Ю.В. Рогов, В.А. Шевченко, А.Э. Тенишев, В.Л. Уваров

На основе транспортного кода PENELOPE-2008 разработаны три базовых комплекса программ для моделирования процессов воздействия сканирующего пучка электронов на объекты различной геометрии и из разных материалов. Для тестирования разработанных программ на их основе были рассчитаны пробег и удельные потери энергии электронов, а также массовый коэффициент ослабления фотонов в различных средах в диапазоне энергии частиц 1…30 МэВ. Проведено сравнение полученных результатов с референтными данными, содержащимися в докладе 35 МКРЕ. На втором этапе валидации были проделаны расчет и измерение поглощенной дозы в стандартном полистирольном калориметре, а также ее распределений в прямоугольном фантоме, перемещаемых через зону воздействия сканируемым пучком электронов. Применение разработанного ПО обеспечивает возможность анализа и оптимизации режимов промышленной обработки продукции на ускорителе электронов.

РОЗРОБКА ТА ВАЛІДАЦІЯ ПРОГРАМНОГО ЗАБЕЗПЕЧЕННЯ ДЛЯ МОДЕЛЮВАННЯ РЕЖИМІВ ОБРОБКИ ПРОДУКЦІЇ НА ПРИСКОРЮВАЧІ ЕЛЕКТРОНІВ

В.І. Нікіфоров, М.М. Пеліхатий, Р.І. Помацалюк, Ю.В. Рогов, В.А. Шевченко, А.Е. Тєнішев, В.Л. Уваров

На основі транспортного коду PENELOPE-2008 розроблено три базові комплекси програм для моделювання процесів дії скануючого пучка електронів на об'єкти різної геометрії і з різних матеріалів. Для тестування розроблених програм на їх основі були розраховані пробіг і питомі втрати енергії електронів, а також масовий коефіцієнт ослаблення фотонів у різних середовищах у діапазоні енергії частинок 1…30 МеВ. Проведено порівняння отриманих результатів з референтними даними, що містяться в доповіді 35 МКРО. На другому етапі валідації були виконані розрахунок і вимірювання поглинутої дози в стандартному калориметрі з полістиролу, а також її розподілів в прямокутному фантомі, переміщуваних через зону дії скануючим пучком електронів. Застосування розробленого ПО забезпечує можливість аналізу та оптимізації режимів промислової обробки продукції на прискорювачі електронів.