MODIFICATION OF THE PENELOPE TRANSPORT SYSTEM FOR HS SIMULATION OF ISOTOPE PRODUCTION MODE

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Abstract

A method has been developed for high-speed computing the photonuclear isotope yield along with the absorbed radiation power in exit devices of electron accelerator. The technique involves a step-by-step calculation of isotope microyield along the photon trajectories. The approach has been realized in the computer programs based on the PENELOPE system of -2001, -2006 and -2008 versions. For their benchmarking, use has been made of the experimental data on activity distributions of the ^{67}Cu produced from ^{68}Zn(γ,p)^{67}Cu reaction in thick zinc targets. The results of simulation using the PENELOPE-2006 and -2008 codes are in excellent agreement with all experimental data. At the same time, the PENELOPE-2001 computations give good agreement with the experimental results for target activation by electron beam, but systematically underestimate (~15%) in case of the target exposed to bremsstrahlung. The proposed technique provides a ~ 10^4 times higher computation speed as compared with the direct Monte Carlo simulation of photonuclear events and that speed is independent of the reaction cross section.

INTRODUCTION

The calculation of the photonuclear isotope yield from a thick production target exposed to a substantially nonuniform mixed flow of electrons and bremsstrahlung photons is a rather complicated task. The problem is best solved with the computer simulation based on the Monte Carlo (MC) transport systems MCNP [1], PENELOPE [2], etc. It should be noted that the PENELOPE simulates only electromagnetic processes, while the MCNP also enables the computation of neutron and proton transport.

The validity of simulation results is determined by the accuracy of particle transport calculation as well as the reaction cross section description. At the same time, the application of even validated codes for the solution of the problem gives sometimes a disagreement (up to 50% and more) with the experimental data (e.g., see [3, 4]). In case of a great amount of computations (in particular, in the optimization problems) apart from the accuracy of the method, its speed of operation is also of importance.

The PENELOPE code in its basic package provides simulation of electron, positron and photon cascades. To determine the isotope yields, we have modified the package by adding the algorithms of two essentially different computing methods. This report presents the description as well as the comparative analysis of both the accuracy and the operating speed of the developed methods.

CALCULATION TECHNIQUE

The simulated trajectory of the photon of initial energy k in the target presents a sequence of linear segments (steps) between the points of its interaction with atoms. The length l_s of each s-step of the photon trajectory in the target randomly varies in the neighborhood of the free path value $r(k)$ or

$$l_s \sim r(k) = \mu^{-1}(k) \quad , \tag{1}$$

where $\mu(k)$ is the photon attenuation coefficient [5]. To determine the isotope yield, at the end of each step the probability of a single photonuclear reaction is calculated through the comparison of the reaction cross section with the cross sections for all other electromagnetic interactions of the photon – the Direct Simulation of Events (DSE) method. It should be noted here that the contribution of photonuclear processes to the total cross section is generally no more than several percent [5].

The photon energy k_s along each s-step of its trajectory may be assumed to be constant. Therefore, the total isotope yield Y can be represented as a sum of microyields from all the steps along the trajectories of all the photons that have crossed the target in any direction, wholly or in part, or have been produced in it. Then Y may be written as

$$Y = \sum_s (1 - e^{-n_A \cdot \sigma(k_s) \cdot l_s}) \, , \tag{2}$$

where n_A is the density of the target nuclei, $\sigma(k_s)$ is the reaction cross section for the photon of energy k_s - the Step-By-Step Microyield (SBSM) method.

RESULTS AND DISCUSSION

Benchmark Experiment

To estimate the programs developed, we have performed computations by the both methods to calculate the spatial distribution of the ^{67}Cu produced from the ^{68}Zn(γ,p)^{67}Cu reaction at different target photoactivation conditions. The reaction cross section has been taken from the reference data [6].

The simulation conditions corresponded to the experiment described in ref. [3]. Namely, two configurations of the output devices of the accelerator were reproduced: i) as a target directly exposed to accelerated electrons, and ii) with an intermediate target-converter of bremsstrahlung. Each target presented a parallelepiped consisting of closely stacked 36 square

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plates from natural zink, 50.8 mm in width and 1.59 mm in thickness.

A direct target activation was achieved with the electron beam (55 MeV, 4μA). In case of bremsstrahlung activation, the converter was exposed to the (49Mev, 100 μA) electron beam. The target exposure time was 40 min. in both cases. The experimental data for the ^{67}Cu activity distribution in separate Zn plates along the axis of the target under its activation by electrons and bremsstrahlung photons have been presented in refs. [3] and [7], respectively. The total uncertainty of activity measurements was estimated to be 10%.

Comparison with Experimental Data

Fig.1 shows the experimental data on ^{67}Cu activity distribution along the target axis at EOB, and also the results of simulation with the use of the DSE and the PENELOPE of -2001 and -2006 versions. As in ref. [3], the final value of the activity produced was normalized to 1 MJ of the electron beam energy.

Simulation with the use of the given algorithm and the PENELOPE-2008 has resulted in the data fully coincident with the ones obtained on the basis of the -2006 version.

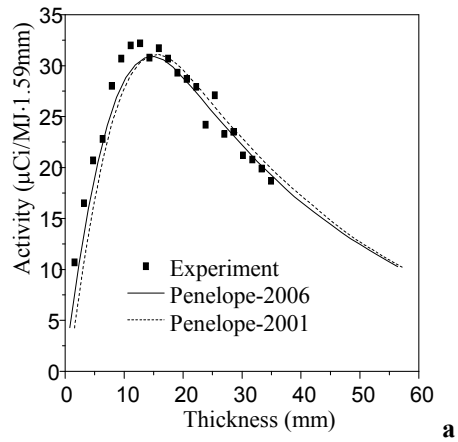

Figure 1: ^{67}Cu isotope activity distribution measured and calculated by the DSE: a) electron beam; b) bremsstrahlung.

The results of the SBSM simulation using the PENELOPE-2008 are presented in Fig.2. In particular, the computations show that the photons leaving the converter have an average exit angle of about 17 degrees. Therefore, the converter-target distance d exerts an essential effect on the value of activity produced in the target. Thus, curves 1 to 4 in Fig. 4b correspond to d = 75, 40, 20 and 0 mm, respectively. It can be seen that the maximum yield is attained at d = 0 mm. In this case, the total target activity is 68% higher than the value obtained in the experiment.

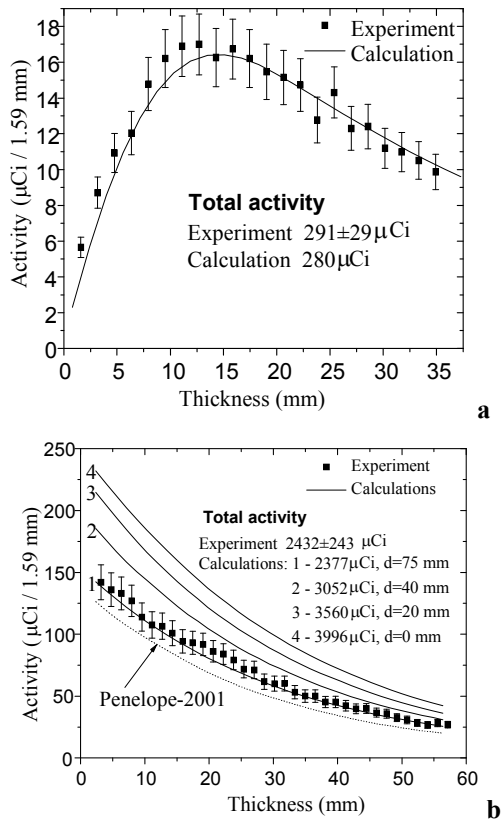

Figure 2: Activity distribution in the zinc target under irradiation with: a) direct electron beam; b) bremsstrahlung (SBSM method).

We have also performed similar computations by the SBSM method with the use of earlier PENELOPE of -2001 and -2006 versions. Comparison between the obtained results (see Fig. 3) testifies that as in the case of application of the DSE method, all the programs provide good description of activity distribution in the target as it is exposed to a direct electron beam (Fig. 3a). As to the case of activation by bremsstrahlung (Fig. 3b), the data obtained with the versions PENELOPE-2006 and -2008 are practically coincident and show very close agreement with the experimental results. On the other hand, the application of the PENELOPE-2001 for modeling of the bremsstrahlung activation by both methods gives the same underestimated (by ~ 15%) result (see Fig. 1).

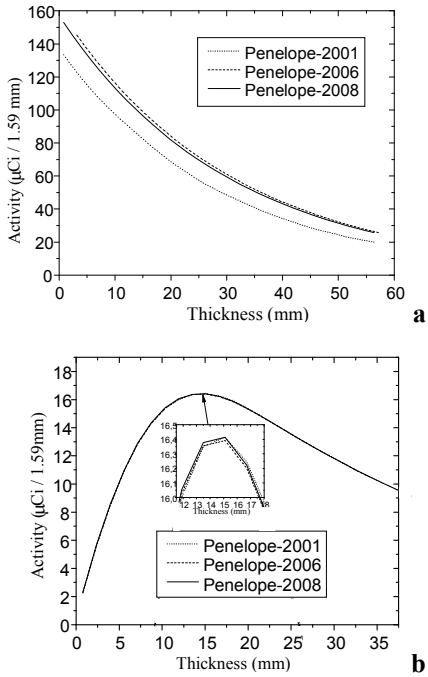

Figure 3: Comparison of target plate activity distributions computed on the basis of different PENELOPE versions (SBSM method): a) electron beam, b) bremsstrahlung

Comparison of the Efficiency

For comparative estimation of adequacy and efficiency of the DSE and SBSM methods we have performed on their basis a combined simulation of the both modes of target activation using the PENELOPE-2008. The computations were carried out by a PC (3.0 GHz Intel Core 2; 2 GB RAM). The computation time of target activation by the electron beam and by bremsstrahlung was 97 and 87 hours, respectively.

The simulation data are presented in Table 1. The latter gives the number of events of ^{67}Cu nuclei generation in the target for a period of computation, the normalized nuclear yield per electron of the primary beam, and the statistical uncertainty. The data fit for the total yield of the ^{67}Cu (accurate to 0.2% and 0.4% at direct electron irradiation and under bremsstrahlung, respectively) as well as the agreement between the activity distribution data indicate that the methods are mutually adequate.

Table 1: Characteristics Computation Algorithms

Method	Number of events	Nuclear yield/e$^-$ (10^{-5})
Electron beam activation		
DSE	24601	7.708±0.034
SBSM	24545	7. 690±0.00039
Bremsstrahlung activation		
DSE	9781	2.043±0.062
SBSM	9824	2.052±0.00043

The efficiency (operating speed) of the methods was estimated by comparing their computation time required to provide the identical statistical uncertainty of simulation results. As is seen from the data given in Table 1, in the case of target exposure to a direct electron beam the SBSM technique appears more efficient than the DSE by a factor of 7569. In simulation of target activation by the bremsstrahlung, the SBSM method appears more efficient than the DSE by a factor of 20736. That is, the result obtained by the DSE for 87 hours is provided by the SBSM calculation in 15 seconds. For example, the time of SBSM-based computation of curves 1 to 4 in Fig.2b ranges from 10 to 30 min. at a statistical uncertainty between 0.4 and 0.2%.

CONCLUSION

The two methods developed for calculating the photonuclear yield of isotopes are embedded into the basic package of the MC transport system. Therefore, they make it possible to compute simultaneously not only the isotopic product yield, but also the absorbed radiation power in the exit device components of the accelerator, and hence, enable one to optimize the mode of target activation with due regard for thermal stability of the target. This possibility is of crucial importance in view of the prospects offered by the development of photonuclear technology at high-power electron accelerators (e.g., see [8]).

With the use of PENELOPE-2006 and -2008 codes, the results of simulation based on the developed methods are in good agreement with the experimental data for the both modes of target activation, namely, by the electron beam and the bremsstrahlung. At the same time, the SBSM technique provides a ~ 10^4 times higher computation speed, and in contrast to the DSE, this speed is independent of the reaction cross section.

REFERENCES

[1] J.F.Briesmeister "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5". Tech. Rep. LA-UR-03-1987, LANL, 2003.
[2] F.Salvat, J.M.Fernández-Varea and J.Sempau "PENELOPE–2008. A Code System for Monte Carlo Simulation of Electron and Photon Transport". OECD, NEA, Issy-les-Moulineaux, France, 2008.
[3] Y.Danon et al., NS Trans. 98 (2008) 894.
[4] K.Kosako et al., J.Nucl.Sci.Technol. 47 (2010) 286.
[5] I.H.Hubbel. Jnt.J.Appl.Rad.Isot. 33 (1982) 1269.
[6] Handbook of photonuclear data for applications: Cross sections and spectra, IAEA-TECDOC-1178, IAEA, 2000.
[7] N.I.Ayzatskiy et al., Probl.Atom.Sci.Technol. Ser.:Nucl.Phys.Inv. 3 (2008) 194.
[8] S.Koscnielniak et al., "Proposal for a ½ MW Electron Linac for Rare Isotope and Materials Science". EPAC'08, Genova, June 2008, p.985 (2008); http:www.JACoW.org.