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X-ray simulation with the Monte Carlo code PENELOPE. Application to Quality Control.

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Abstract— **A realistic knowledge of the energy spectrum is very important in Quality Control (QC) of X-ray tubes in order to reduce dose to patients. However, due to the implicit difficulties to measure the X-ray spectrum accurately, it is not normally obtained in routine QC. Instead, some parameters are measured and/or calculated. PENELOPE and MCNP5 codes, based on the Monte Carlo method, can be used as complementary tools to verify parameters measured in QC. These codes allow estimating Bremsstrahlung and characteristic lines from the anode taking into account specific characteristics of equipment. They have been applied to simulate an X-ray spectrum. Results are compared with theoretical IPEM 78 spectrum. A sensitivity analysis has been developed to estimate the influence on simulated spectra of important parameters used in simulation codes. With this analysis it has been obtained that the FORCE factor is the most important parameter in PENELOPE simulations. FORCE factor, which is a variance reduction method, improves the simulation but produces hard increases of computer time. The value of FORCE should be optimized so that a good agreement of simulated and theoretical spectra is reached, but with a reduction of computer time. Quality parameters such as Half Value Layer (HVL) can be obtained with the PENELOPE model developed, but FORCE takes such a high value that computer time is hardly increased. On the other hand, depth dose assessment can be achieved with acceptable results for small values of FORCE.**

I. Introduction

The Quality Control (QC) of X-ray tubes in medical radiodiagnostic services is very important to reduce the dose imparted to patients as much as possible. The main objective of QC is to assure the optimum operation of the X-ray tube, which implicitly means to estimate the energy spectrum. The main quality parameters are First and Second Half-Value Layer (HVL), homogeneity factor, and mean energy. They can be obtained from the energy spectrum. A minimum thickness of the inherent filtration in a diagnostic X-ray unit is a requirement to reduce dose to patients [1]. A measurement of the total filtration to ensure compliance with this concept is recommended by ISO [2]. Several indirect methods to determine quality parameters have been proposed [3, 4, 5]. However, all of them contain some uncertainties due to the difficulty to accurately know the X-ray spectrum. Monte Carlo (MC) methods such as PENELOPE [6] and MCNP5 [7] as well as present powerful computer capabilities allow simulating complex geometrical features of the actual tube. Furthermore, they permit to simulate the X-ray spectrum for certain working conditions, being quality parameters associated to X-ray beam also calculated.

In previous works [8, 9], authors developed a MC model using the MCNP5 code to simulate X-ray spectra by means of a point detector (tally F5). This tally represents by itself a variance reduction technique because it makes use of a semi-deterministic algorithm [7]. In PENELOPE, X-ray production is influenced by the choice of certain simulation parameters, some of them related to variance reduction techniques.

The goal of this work is to establish the effect of these parameters on the X-ray spectrum and to determine their repercussion on the imparted dose to patients. A PENELOPE model of a commercial X-ray tube has been developed, simulating different working conditions. For all cases considered, results obtained with PENELOPE have been compared with those from MCNP5 and also with theoretical spectra extracted from the IPEM 78 Report Catalogue [10]. A quantitative comparison between all spectra has been done calculating the Root Mean Squared (RMS) and quality parameters for each working condition. Finally, to estimate the effect on simulated spectrum of a variation on specific PENELOPE parameters, depth dose curves in a water phantom have been calculated.

II. Method

A. X ray simulation with the PENELOPE code

The PENELOPE (PENetration and Energy Loss Of Positrons and Electrons) code allows simulating interactions of different particles (electrons, photons and positrons). Its use is widespread and permits to simulate the Bremsstrahlung continuum and characteristic lines (K- and L- lines) arising from the interaction of electrons with matter [6]. PENELOPE is based on the separation of the collision events respectively

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in hard and soft according to the energy lost and/or the change in the particle direction being larger or smaller than certain cut-off values. Elastic and inelastic electron and positron collisions, Bremsstrahlung emission and positron annihilation are the interaction mechanisms included in the code. For electron interactions, the effect of soft interactions is described using an adequate multiple scattering approximation. Hard interactions, which involve energy transfers or angular deflections larger than the cut-off selected by the user are simulated individually from the corresponding differential cross sections (DCSs) [11]. X-rays are only produced through inner-shell ionisation by electron impact and Bremsstrahlung emission, which occur with very small probabilities. Furthermore, in the X-ray simulation many electron histories are needed to get one emerging photon and only a few emerging photons reaches the detector point. For these reasons, the direct simulation of X-ray spectra is very inefficient.

To achieve a better simulation of electron transport, PENELOPE permits to select appropriate values for cut-offs and other simulation parameters, as well as the use of appropriate variance-reduction techniques [11]. The algorithm is controlled by four parameters:

- C1 gives the average angular deflection due to a hard elastic collision and all previous soft collisions.
- C2 represents the maximum permitted value for the average fractional energy loss in a step.
- W_{CC} is the energy cut-off referred to hard inelastic collisions.
- W_{CR} is the energy cut-off referred to hard Bremsstrahlung emission

The variance-reduction technique, known as the method of weights or interaction forcing, consists in artificially increasing the probability of inner-shell ionisation and Bremsstrahlung emission and, at the same time, assigning appropriate statistical weights to generated secondary photons in such a way that the simulation results remain unbiased. To apply this technique, the user has to specify forcing factors, FORCE (IBODY, KPAR, ICOL, WLOW, WHIGH) [6], where:

- IBODY corresponds to the number of bodies or geometrical cells considered,
- KPAR indicates the type of particle simulated (electrons, photons, positrons),
- ICOL determines the type of collision,
- WLOW and WHIGH represent the fraction of particle weights considered in the following steps after applying the FORCE interaction.

B. The X-ray model

In this paper, the X-ray spectrum has been obtained by tracking a large number of incident electrons hitting the anode until they are absorbed or scattered, and calculating the Bremsstrahlung and characteristic photons produced within the target. The modelled X-ray tube includes a 12º angle Tungsten anode and 4 mm of aluminium filter. It can be seen in Figure 1 the geometrical layout of the system, modelled with SABRINA [12].

The electron emission has been characterized as a point source emitting monochromatic electrons within a solid angle, in void. Electrons impact in a circular area of 1 mm diameter.

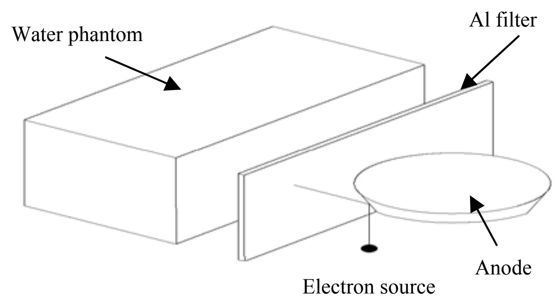

Figure 1. Geometrical layout.

III. RESULTS

A 100 kVp spectrum has been chosen as base case, setting the following values for PENELOPE simulation parameters: C_1 = 0.2; C_2 = 0.2; W_{CC} = 1000 eV; W_{CR} =1000 eV; FORCE = 50. These values have been chosen according to the best results obtained in the sensitivity analysis performed in this paper. Comparison between simulated spectra (PENELOPE and MCNP5 including 3σ error bars) and theoretical spectrum extracted from IPEM 78 is shown in Figure 2.

As it can be seen, both simulated spectra fit successfully the shape of the theoretical distribution (IPEM 78) in the whole energy range. Simulated spectra reproduce accurately characteristic X-rays ($K_{\alpha 1}$ = 59.318 keV, $K_{\alpha 2}$ = 57.981 keV, $K_{\beta 1}$ = 67.245 keV $K_{\beta 2}$ = 69.102 keV and $K_{\beta 3}$ = 66.952 keV) and Bremsstrahlung continuous. However, characteristic lines are underestimated in comparison with IPEM 78. Anyway, PENELOPE improves the height of the characteristic lines respect to MCNP5. Regarding to L lines, they are not present in the spectra due to the added filter of aluminium in the model. In the energy range between 30 and 50 keV, both MCNP and PENELOPE produce a slight overestimation of the Bremsstrahlung continuous, although this overestimation is reduced in the case of PENELOPE. It is observed that MNCP5 3σ error bars are higher than PENELOPE ones for the same number of particles simulated.

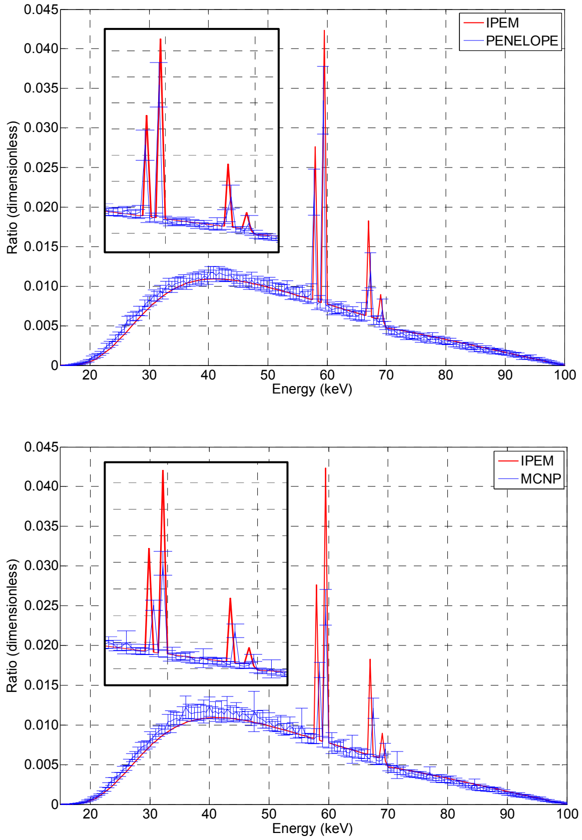

Figure 2. Theoretical and simulated spectra for 100 kVp.

FORCE is one of the most important parameters in PENELOPE for simulation of X-ray spectra. To study the effect on the spectrum of FORCE variation a sensitivity analysis has been performed. Figure 3 shows the spectrum obtained for FORCE = 10. Comparing this Figure with Figure 2a (FORCE = 50) it can be seen that error improves when FORCE is increased. However, the higher the FORCE parameter, the lower the speed simulation ($5.36 \cdot 10^2$, $1.51 \cdot 10^3$ showers/sec for FORCE equal to 10 and 50 respectively).

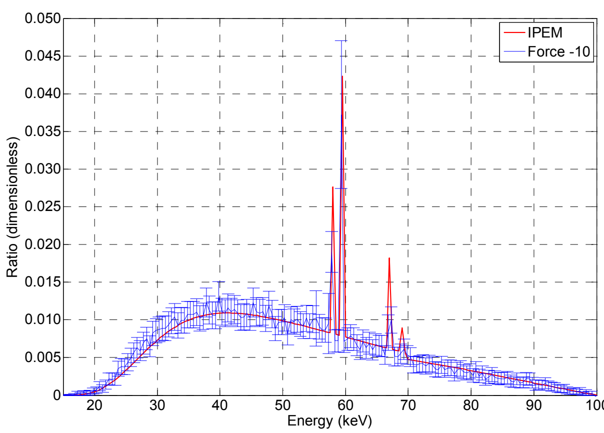

Figure 3. PENELOPE spectra obtained for different FORCE values.

Another sensitivity analysis has been performed varying W_{CC} and W_{CR} in the base case. Results show that their effect is negligible in the continuous Bremsstrahlung when FORCE is activated because 3σ error bars are overlapped. However, to reduce computer time, higher values for W_{CC} and W_{CR} should be chosen.

To assess the deviation of simulated spectra respect to theoretical IPEM spectrum the Root Mean Squared, RMS, has been calculated. Results are listed in Table I for different values of FORCE. When FORCE is increased, RMS decreases, consequently PENELOPE spectra are improved.

Quality parameters have been also calculated for IPEM and simulated spectra. The First HVL of an X-ray beam is defined as the thickness of an absorbing material (aluminium in this case) needed to reduce the air-kerma to 50% of its original value, in narrow beam conditions. The Second HVL is the additional attenuator thickness (aluminium) required to reduce the air-kerma form one half to a quarter. The homogeneity factor is defined as the ratio between first to second HVL. Results are listed in Table I too. Discrepancies between simulated and IPEM spectra produce relative differences in First and Second HVL lower than 7 %. As it can be seen, lower values are also achieved for higher FORCE values.

TABLE I. QUALITY PARAMETERS OF THE BEAM

Spectrum	RMS (%)	Quality parameters			
		1st HVL (cm Al)	***2nd HVL (cm Al)***	***Coef Homog.***	***Mean Energy***
IPEM		0.407	0.997	0.408	52.34
MCNP	4.42	0.389 (4.42)	0.964 (3.31)	0.404 (1.03)	50.94 (2.67)
PENELOPE FORCE 50	4.02	0.386 (5.34)	0.966 (3.11)	0.400 (2.14)	51.18 (2.22)
PENELOPE FORCE 30	4.41	0.386 (5.34)	0.964 (3.31)	0.400 (1.94)	51.17 (2.23)
PENELOPE FORCE 10	4.61	0.381 (6.62)	0.955 (4.21)	0.399 (2.30)	51.02 (2.52)

Relative error respect to IPEM 78 into brackets

To estimate the effect of these discrepancies depth dose curves in a water phantom of 10x10x10 cm^3 have been estimated. The photon transport in air and water has been calculated following individual photon and electron histories throughout the whole geometry. A detailed photon physics treatment, including photoelectric effect with fluorescence production, incoherent and coherent scattering, has been considered in the energy range between 1 and 100 keV.

MCNP5 and PENELOPE calculate dose per emitted particle (electron) at the source. In MCNP5, the Tally F4 (fluence) has been measured in the water phantom and converted into dose using conversion factors of photon fluence to dose extracted from the National Institute of Standards and Technology (NIST) [13].

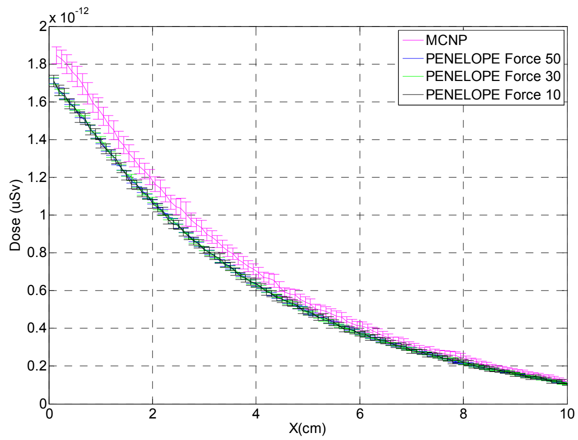

Figure 4. Depth dose curves obtained for MNCP and PENELOPE spectra.

Depth dose curves obtained are shown with their 3σ error bars in Figure 4. As it can be seen, doses and errors are higher for MCNP5 than for PENELOPE mainly at the surface of the water phantom. It can be attributed to the method used by PENELOPE to estimate the mass energy-absorption coefficient. On the other hand, there are no significant differences between depth dose curves obtained with PENELOPE for different values of FORCE. Therefore, it can be chosen a lower FORCE value when dose calculations are concerned, saving hence computer time.

From these results, it has been stated that the appropriate value of FORCE is an intermediate value (FORCE = 30) because it produces acceptable RMS (< 4.5%), Quality parameter errors lower than 5% and relatively low computer time. Furthermore, it has been tested that with this value, depth dose curves and their corresponding 3σ error bars are similar to dose obtained with other FORCE values studied.

IV. Conclusion

Monte Carlo codes, PENELOPE and MCNP5, have been applied to obtain spectra of X-ray tubes. Results are compared with theoretical spectra extracted from IPEM 78. A sensitivity analysis has been developed to estimate the influence on simulated spectra of important parameters used in simulation codes. In particular, FORCE factor in PENELOPE has been analyzed. It is a variance reduction method that, but produces hard increases of computer time.

The value of FORCE should be optimized so that a good agreement of simulated and theoretical spectra is reached, but with a reduction of computer time.

Quality parameters such as HVLs can be obtained with the PENELOPE model developed, but FORCE takes such a high value that computer time is hardly increased. On the other hand, depth dose assessment can be achieved with acceptable results for small values of FORCE. Hence, a shorter computer time.

Therefore, the importance of using an appropriate value of FORCE for Quality Control calculations has been highlighted with the analysis performed.

Concerning dose calculations, a lower FORCE value can be used, saving computer time without significant discrepancies in results.

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