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Uncertainty Analysis in the Simulation of X-ray Spectra in the Diagnostic Range using the MCNP5 code

S. Gallardo, A. Querol, J. Ródenas and G. Verdú

Abstract— **An accurate knowledge of the photonic spectra emitted by X-ray tubes in radiodiagnostics is essential to better estimate the imparted dose to patients and to improve the image quality obtained with these devices. In this work, several X-ray spectra have been simulated using the MCNP5 code to simulate X-ray production in a commercial device. To validate the Monte Carlo results, simulated spectra have been compared to those extracted from the IPEM 78 database. The uncertainty associated to some geometrical features of the tube and its effect on the simulated spectra has been analyzed using the Noether-Wilks formula. This analysis has been focused on the thickness of collimators, filters, shielding and barrel shutter. Furthermore, results show that the uncertainty due to geometrical parameters (0.98% in terms of Root Mean Squared) is higher than the statistical uncertainty associated to the MCNP5 calculations.**

I. INTRODUCTION

ACCURATE experimental measurements of X-ray spectra in the radiodiagnostic energy range present important difficulties especially due to the high fluence rate of photons. The Monte Carlo (MC) simulation of X-ray spectra can be extremely useful for the characterization of actual spectra. The MCNP5 code [1], based on the MC method, is suitable to simulate the production of X-ray spectra and to investigate the effect of the different uncertainties of the calculation in the simulated spectra. In this work, an MCNP5 model reproducing a commercial X-ray tube has been developed, including all parts of the tube, specially: anode, collimators, shielding, beryllium and aluminum foils.

Simulated spectra have been compared with X-ray spectra extracted from IPEM Report 78 catalogue [2]. This database permits to obtain different spectra varying working conditions such as anode material and angle, filter material and thickness, and voltage ripple. Voltage has been varied for calculations from 60 kVp up to 150 kVp.

Most of the experimental and computational investigations, especially those published prior to 1999, failed to include a rigorous uncertainty analysis It is due that there were not clear recommendations about how to do this analysis before 2004, when the American Association of Physicists in Medicine (AAPM) presented their report based on the best estimate uncertainty analysis [3]. In this work an evaluation of some geometrical parameters of an X-ray device is done by MCNP5 simulation to perform an uncertainty analysis. A sampling has been determined by the characteristics of the tolerance intervals by applying the Noether-Wilks formula [4]. A number of simulations equal to the sample size have been carried out modifying the geometrical parameters with uncertainties.

II. METHOD

A. The MCNP5 code

MCNP5 is a general-purpose MC code that can be used for neutron, photon and electron or coupled neutron/photon/electron transport [5]. The code treats an arbitrary three-dimensional configuration of materials in geometric cells. For simulation of X-ray spectra, MCNP5 has been run in photon and electron mode (mode: P, E). To improve the efficiency of electron and photon transport, two cards (PHYS: P and PHYS: E) are considered in MCNP5 for biasing some physical parameters such as production of secondary electrons by photons (IDES), coherent scattering (NOCOH), bremsstrahlung angular distribution (IBAD) and production of characteristic x-rays (XNUM).

A continuous slowing down model is used for electron transport. For photon transport, the code takes into account incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption and bremsstrahlung. To follow an electron through a significant energy loss, the MCNP5 code breaks the electron's path into many steps. One way to achieve acceptable computing times is to reduce the time spent on tracking electrons. This can be done by increasing the cut-off energy for electrons, so the value of this cut-off in MCNP5 has been modified for these calculations.

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MCNP5 is suitable for modelling the flux at a point (tally F5) emitted by the X-ray tube using a semi-deterministic method to improve the variance of results. According to the MCNP5 user manual, the F5 tally requires a statistical uncertainty lower than 5% to produce a generally reliable confidence level [5].

B. *Simulation of X-ray spectra*

The procedure to simulate X-ray production consist in tracking a large number of incident electrons on the tungsten anode target until they are absorbed or emerge from it. The electron source, which has been defined as a point source, emits electrons with a given energy within a solid angle ψ. The electric field has not been simulated, so the maximum energy reached by electrons is the energy specified in the source definition. Electrons hit the anode target at an incident angle of $\theta = 22^{\circ}$ and the full emergent beam angle is about 40º. The simulated X-ray spectrum has been recorded at the exit of the tube using an F5 tally. An X-ray tube whose main features are: tungsten anode, 22º anode angle, 2.2-mm Beryllium and 3.5-mm Aluminum of inherent filtration has been simulated by MCNP5. The layout of the tube is shown in Figure 1.

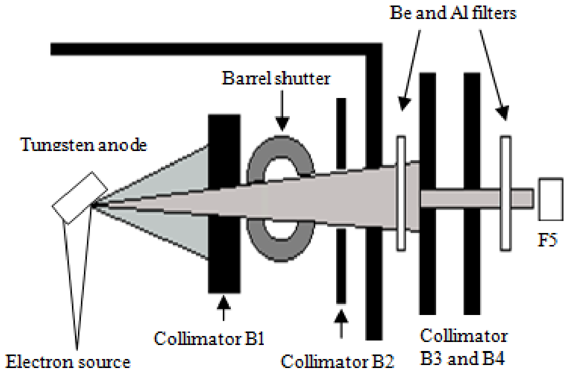

Fig. 1. Layout of the simulated X-ray tube.

A. *Uncertainty analysis*

In an MCNP5 simulation, uncertainties can be attributed to different causes. Attending these causes, the MCNP5 simulation uncertainties can be divided in three types:

1) Statistical: due to the stochastic nature of the MC method and the finite number of simulated events.

2) Input: due to the input parameters such as density, geometrical dimensions and material composition.

3) Physics: due to any systematic difference between the way the simulation models radiation interactions with matter and the way these interactions are observed.

The simulation uncertainty may be expressed as it is shown in equation 1.

$$u^2_{simulation} = (u^2_{statistic} + u^2_{inputs} + u^2_{physics}) \quad (1)$$

The uncertainty due to the systematic difference between the physics model and measurements has been neglected in absence of any experimental data, which the calculated results can be directly compared with [6].

Regarding the statistical uncertainties, they are given by the MCNP5 code along with results of calculations.

This work is focused on the study of the influence of input uncertainties on the X-ray simulated spectra using the MCNP5 code. Several geometrical variables have been varied, according to their uncertainty. Table I contains a list of all parameters varied during simulations.

One important phase is the assignment of the so-called Subjective Probability Distribution Function (SPDF) to quantify the uncertainty of the X-ray tube geometric parameters listed in Table I. to

TABLE I
LIST OF PARAMETERS STUDIED

Parameter	Value (mm)
Thickness Pb collimator B1	35 ± 10
Thickness Pb shutter	5 ± 1
Thickness Pb collimator B2	6 ± 1
Thickness Pb shielding	8 ± 1
Thickness Be filter	2.2 ± 0.7
Thickness Pb collimator B3	6 ± 1
Thickness Pb collimator B4	6 ± 1
Thickness Al filter	3.5 ± 1

The selection of these functions is the most subjective part of the methodology as the SPDFs reflect how well the uncertainty in input parameters is known. In this work, it has been assumed that all the parameters listed in Table 1 follow a normal distribution. As the precision of manufacturing is not known, a large variation has been chosen for all the input parameters studied.

The process starts with the generation of a random sample of input parameters, according to the SPDFs assigned to them. The minimum number of MNCP5 simulations is given by the formula of Wilks [4, 7], and according to the degree of precision desired for uncertainty measures. Thus, the number of required calculations does not depend on the number of input parameters or on any assumption about the probability distribution of results [8]. A tolerance defined in the interval between a lower (L) and upper (U) limit is an estimation of a random variable that contains a specified fraction of the variable probability, p, with a prescribed level of confidence, γ [9]. Tolerance intervals are constructed from sampled data so as to enclose p% of the population of a random variable X with a given confidence γ.

If a random sample of output values has a normal PDF, it is possible to compute tolerance intervals from the sample mean, m_y, and sample standard deviation, s_y as it is shown in equation 2:

$$(L, U) = (m_y - Ks_y, m_y + Ks_y) \quad (2)$$

where K is the tolerance factor, whose values depend on the sample size, probability coverage, p, and confidence level, γ. The values for K are tabulated for different p, N and γ in standard statistical tables [9, 10]. To estimate the tolerance interval with a 95% of confidence level the minimum number of MCNP5 simulations required is 93.

III. RESULTS AND DISCUSSION

Spectra obtained by MCNP5 simulations have been compared with the corresponding spectra of IPEM 78. Simulations have been done for several tube voltages in the radiodiagnostic range (from 60 up to 150 kV). In Figure 2 it is shown the comparison between theoretical and simulated spectra for 150 kV.

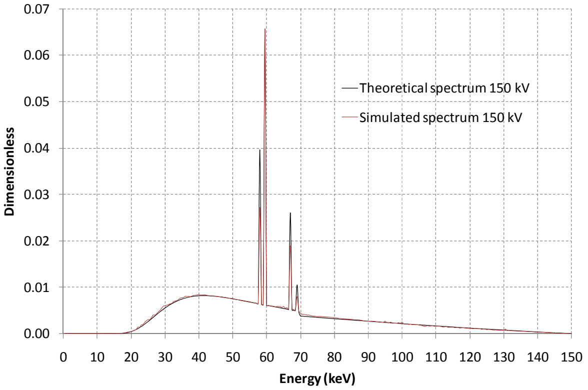

Fig. 2. Theoretical and simulated spectrum for 150 kV.

To have a quantitative understanding of the deviation of the simulated spectra from the theoretical IPEM spectrum, the Root Mean Squared (RMS), have been calculated to estimate the good quality of fitting, according to equation 3.

$$RMS=\frac{\sqrt{\frac{\Sigma(x_{theoretic}-x_{simulated})^2}{n}}}{x_{simulated_{max}}}\cdot 100 \qquad (3)$$

This method is used to evaluate whether or not the observed variations in the simulated spectrum are within an acceptable range.

It can be seen in Figure 2 that MCNP5 simulation has good agreement with IPEM report with small differences visible in the intensity of characteristic lines. These differences give a RMS value of 0.74. This underestimation is consistent with the fact that characteristic photons in MCNP5 are created by an electron impact ionization (EII) process. This is regulated by the parameter XNUM on the PHYS: E card, which is used to control the sampling of X-ray photons produced along electron substeps [11, 12]. Despite underestimation in tungsten characteristic lines, the spectrum generated by MCNP5 can be considered a good agreement with IPEM 78 spectrum.

The uncertainty analysis is based on a sample of 93 MCNP5 simulations, sufficient to guarantee double tolerance limits as explained in Section II. Simulations have been performed for a 150-kV voltage varying the input variables shown in Table 1.

It can be seen in Figure 3, the simulated spectrum obtained for 150 kV and the upper and lower limits corresponding to the statistics uncertainty (2σ). A zoom of the differences between spectra due to the statistical MCNP5 uncertainties is shown at the right corner.

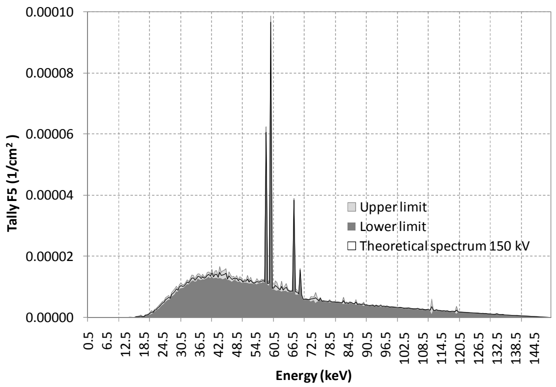

Fig. 3. Simulated spectrum with MCNP5 uncertainty.

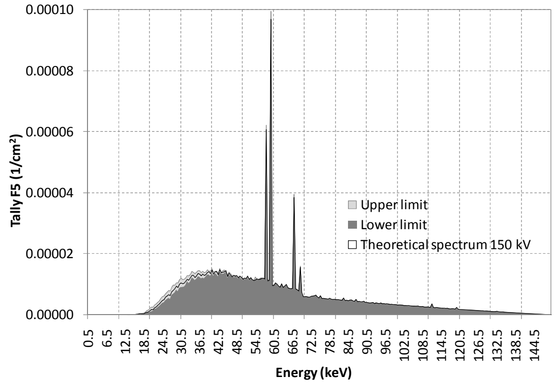

Fig. 4. Theoretical and simulated spectra for maximum and minimum RMS.

In Figure 4 it is shown the tolerance (low and upper limits) obtained using the Wilks methodology explained in Section II. The most important differences are observed in the low energy range. A zoom of this range is shown at the right corner of the Figure 4.

As the uncertainty of the physics component has been neglected, the MCNP5 simulation uncertainties can be obtained by the composition of the statistical and inputs uncertainties shown in Figures 3 and 4.

Uncertainty associated with the input parameters was found to be greater than MCNP5 statistical uncertainty. The highest difference between upper and lower limit considering MCNP5 statistical uncertainty is $4.86\cdot10^{-6}$ ($1/cm^2$) while in the input uncertainty case this value is 6.38 10^{-6} ($1/cm^2$). It is important to remind that all results are given per particle emitted by the source.

On the other hand, Quality Parameters (QC) such as first and second half value layer (HVL), homogeneity factor and mean energy have been calculated for both theoretical and simulated spectra. Normally, the HVL is experimentally obtained by overlapping aluminum or copper foils of certain thickness and certified purity between the X-ray focus and an ionization chamber. However, HVL can also be determined by calculation if the primary X-ray spectrum is known [13, 14, 15].

Reducing the air kerma to 1/4, the second HVL can be obtained. Homogeneity factor is defined for each voltage as the ratio between the first and the second HVL. For a given photon spectrum the mean photon energy is an important parameter because it represents the chromatic quality of the spectrum.

RMS and QP have been calculated for each of the 93 simulations proposed. In the Table II, only results of cases corresponding to the maximum (#58) and minimum (#87) RMS are listed. Relative errors (in %) between simulated and IPEM78 spectra appear into brackets.

TABLE II
QUALITY PARAMETERS AND ROOT MEAN SQUARED

	1st HVL (mm Al)	2nd HVL (mm Al)	Mean Energy (keV)	Hom. Factor	RMS (%)
Case #58	0.474	1.229	59.78	0.386	0.99
	(-8.14)	(-5.97)	(-1.63)	(-2.31)	
Case #87	0.549	1.366	61.54	0.402	0.79
	(6.40)	(4.51)	(1.27)	(1.80)	
Theoretical	0.516	1.307	60.77	0.395	

Furthermore, a sensitivity analysis has been done to study the effect of each input parameter separately. RMS values obtained for maximum and minimum variation of each input parameter are shown in Table III.

TABLE III
ROOT MEAN SQUARED VARYING EACH PARAMETER

Collimator B1 (mm Pb)	RMS (%)	Barrel Shutter (mm Pb)	RMS (%)
25	0.81	4	0.80
45	0.79	5	0.79

Collimator B2 (mm Pb)	RMS (%)	Shielding (mm Pb)	RMS (%)
5	0.81	7	0.80
7	0.79	9	0.79

Filter Thickness (mm Be)	RMS (%)	Collimator B3 (mm Pb)	RMS (%)
1.5	0.80	5	0.81
2.9	0.77	7	0.79

Collimator B4 (mm Pb)	RMS (%)	Filter Thickness (mm Al)	RMS (%)
5	0.81	2.5	0.98
7	0.79	4.5	0.80

RMS values obtained only considering aluminium variation are higher than those obtained varying the other input parameters. At the same time RMS values for varying only the aluminium thickness are close to those obtained from the global input uncertainty, listed in Table II.

This fact permits to conclude that the parameter with higher relevance is the uncertainty due to the aluminium thickness, despite the large uncertainty associated with all the input parameters studied in this work.

From the results obtained in this work, it can be said that the methodology exposed in this paper can be extrapolated to a conventional clinical imaging system. To achieve this, it would be required a MCNP5 model of the X-ray tube used and a sensitivity analysis would be performed studying some of its dimensional parameters. The results of this study would give the most influential parameters in the MCNP5 global simulation uncertainty.

IV. CONCLUSION

An MCNP5 model has been validated to simulate X-ray spectra in radiodiagnostic energy range.

Results have proved that the statistical uncertainty due to the stochastic nature of the MC method is less important than the uncertainty due to the geometrical parameters analyzed.

The results obtained in the sensitivity analysis shown that aluminium filter thickness is the most important contributor to the total uncertainty in MCNP5 simulations.

The effect of simulation uncertainties on the total uncertainty is small but non-negligible; therefore, it should be taken into account when possible.

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