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Research Article

An Intercomparison Exercise Between EGSnrc and MCNPX for Validation of New *egs_kerma* User Code

L. F. Araujo[*,1], C.V.G. Ferreira[1], F.S.G. Silva[1], L. Paixao[2], T.C.F. Fonseca[1]

[1] *Department of Nuclear Engineering - DEN, UFMG, BH 31270-901, MG, Brazil.*

[2] *Department of Anatomy and Image - FM, UFMG, BH 30130-100, MG, Brazil.*

E-mail* :*lucasfaraujo@ufmg.br (corresponding author);*

ORCID:0000-0001-6837-6213

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ABSTRACT:
Background: The "Case 1" exercise described in the TG report 195 of the American Association of Physicists in Medicine was used. This exercise aims to verify the material attenuation of a filter of aluminum and the half and quarter-value layer calculations.
Purpose: The objective of this work was to perform an intercom-parison exercise using two Monte Carlo codes, MCNPX and EGSnrc, and its recently released *egs_kerma* user code.
Method:A collimated X-ray source was considered for two mono-energetic (30 and 100 keV) and two X-ray spectra (30 kVp Mo/Mo and 100 kVp W/Al) beams.
Results: The HVL and QVL results obtained using both MC codes were compared to the results provided by the TG 195. The average percentage deviations obtained between the results and the pub-lished by TG 195 were less than 1% for both sources.
Conclusions: The results obtained between the MC codes were used to validate the newly released *egs_kerma* user code, which com-pared to cavity user code results have shown no differences.
Keywords: Computational Modelling, Monte Carlo Simulation, egs kerma, TG 195, EGSnrc, MCNPX.

1. Introduction

Simulations with Monte Carlo (MC) computational codes are widely used in medical physics, due to its ability to reproduce experimental practices and accurately estimating the interaction of ionizing radiation with matter [1] - [5]. MC codes such as the Electron Gamma Shower of the National Research Council (EGSnrc) and Monte Carlo N-Particle Transport Code eXtended (MCNPX) are well known and robust MC packages [2, 5]. One important task when using an MC code to perform a computational experiment is the validation step. This validation will ensure that the MC codes present reliable and accurate results and check out the researchers for knowledge about the physics and geometry modelling of the experiment [6]. The validation can be performed by reproducing computationally using an MC code a computer experiment already published and fulfilled with a validated MC code [7]. If the results obtained in the validation are similar to those of the reproduced experiment or within the deviation expected, the code will be considered validated.The TG-195 report provides a common reference for bench-marking the Monte Carlo simulations which cover a range of MC codes and different scenarios [7]. This type of report is very useful for the scientific community and it can be used to show how to perform, for different MC codes, the modelling and simulation of a series of exercises already validated. The report provides a data set in which allows performing the simulation for example, a case of diagnostic medical imaging

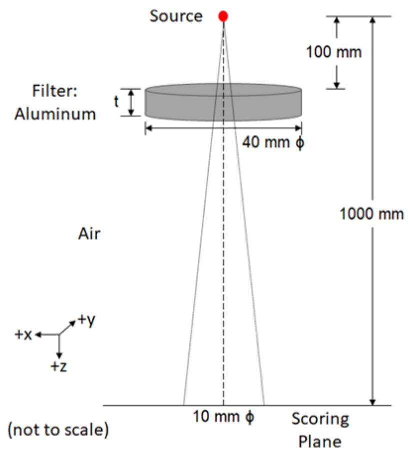

Figure 1: Geometry model proposed in the "Case 1" of TG 195 report. Source: AAPM TG-195[7].

and low X-ray energies. In this paper is reported the exercise "Case 1" provided by the TG-195 [7]. It was modelled and simulated using two MC codes, EGSnrc and MCNPX and it also includes the new *egs_kerma* user code released in 2020. The exercise aims to verify the accuracy of the X-ray spectra sources, the material attenuation by calculating the half and quarter value layers for two monoenergetic (30 and 100 keV) and two X-ray spectra (30 kVp Mo/Mo and 100 kVp W/Al).

2. Method & Materials

2.1. Geometry Modelling

Figure 1 shows the geometry model proposed in "Case 1" of the TG-195 report [7]. The geometry of the model consists of a point source placed at 100 mm from the attenuating filter and 1000 mm from the scoring plane. The X-ray source was collimated to a central circle of 1 mm diameter at the superior face of the filter which gives 10 mm diameter at the scoring plane. The aluminum filter is a disk geometry of 40 mm diameter and two different thicknesses (t) were used to calculate the AK ratio for the half value layer (HVL) and quarter value layer (QVL). Table 1 shows the X-ray energy/spectrum and the aluminum filter thicknesses used for both, HVL and QVL, in the MC simulations and provided in the exercise. The density and material composition parameters of the material used in the simulations were taken from the National Institute of Standards and Technology (NIST) [8]. Validation simulations were performed for two mono-energetic photon sources of 30 and 100 keV and two X-ray spectra of 30 kVp Molybdenum/Molybdenum (Mo/Mo) and 100 kVp Tungsten/Aluminum (W/Al) target/filter combinations. The tabulated spectra were described as probability distribution functions with 0.5 keV energy bin width and also provided in the exercise. The photon fluence was obtained in the scoring plane with and without the attenuation filter. Two different conditions were performed. First for primary (non-scattered) photon fluence and second for primary and the scattered photon fluence. The AK values are calculated from photon fluence using the following equation.

$$AK = E\phi \times \left(\frac{\mu_{\text{en}}}{\rho}\right) \tag{1}$$

where E is the mid-point energy bin, Φ is the fluence at energy bin E and μ_{en} per ρ the air mass energy absorption coefficient. The air mass energy absorption coefficients were provided in the electronic resources of the report. The coefficients for the X-ray energies below 3.75 keV were ignored [7].The HVL and QVL are calculated by the AK ratios as described by the TG-195 (R_1, R_2, R_3andR_4) using different filter thicknesses according to the following equations:

$$R_1 = \frac{\sum_E AK_{\text{P(E, t= HVL)}}}{\sum_E AK_{\text{P(E, t= 0)}}} \tag{2}$$

$$R_2 = \frac{\sum_E AK_{\text{P(E, t= QVL)}}}{\sum_E AK_{\text{P(E, t= 0)}}} \tag{3}$$

$$R_3 = \frac{\sum_E (AK_P + AK_S)_{\text{(E, t= HVL)}}}{\sum_E (AK_P + AK_S)_{\text{(E, t= 0)}}} \tag{4}$$

$$R_4 = \frac{\sum_E (AK_P + AK_S)_{\text{(E, t= QVL)}}}{\sum_E (AK_P + AK_S)_{\text{(E, t= 0)}}} \tag{5}$$

where AKP is related to the primary (non-scattered) photon fluence and the AKS is related to the scattered photon fluence. The following MC codes were used for the modelling and simulations, the MCNPX version 2.7 and the EGSnrc using the cavity and *egs_kerma* user codes. The *egs_kerma* is a new used code tool added

Table 1: Filter thickness (mmAl) for different X-ray energy/spectrum.

	Thickness	
X-ray Energy/ Spectrum	**HVL (mmAl)**	**QVL (mmAl)**
30 keV	2.273	4.546
100 keV	15.110	30.220
30 kVp	0.3431	0.7663
100 kVp	3.950	9.840

Table 2: Checklist of EGSnrc and MCNPX [14].

	Description		
Item Name	**EGSnrc**	**MCNPX**	**References**
Code, version/year	EGSnrc, 2020	MCNPX, 2.7.0, 2011	[9, 11]
Cross-sections	xcom: Rayleigh, photoelectric, and pair production. RIA:Incoherent scattering	ENDF/B-VI: Rayleigh, photoelectric and Incoherent scattering	[9, 11]
Transport Parameters	Charge=0, ECUT=1 and PCUT=0.001,user code cavity and user code *egs_kerma*	Photons cutoff=1×10^{-3} MeV Mode Card=P and PHYS Card=Default	[7]
VRT	Photon splitting	Next Event Estimation	[9, 11]
Scored quantities	Fluence ($cm^{2*}MeV^1$)	Fluence (cm^2)	[9, 11]
Histories	2 ×10^6 particles	5 ×10^8 particles	[9, 11]
Uncertainties		Less than 1%	[7]

to EGSnrc and it was also tested for the Air Kerma (AK) calculations. Table shows the main features used in the simulations.

2.2. EGSnrc

The Electron Gamma Shower of the National Research Council (EGSnrc) is a computational code based on the Monte Carlo mathematical method. It allows the electrons and photons transport in an arbitrary 3D geometry modelled with different materials [9]. It is an adaptive code for any operating systems and distributed as free software for research purposes. The modelling and simulations were performed using the EGSnrc, cavity and *egs_kerma* user codes, released version in an Intel Core $i3-6006UCPU@2.00GHzx4$ and HD Graphics 520 (SKLGT2) using the OS Linux Ubuntu 20.10 (Groovy Gorilla). The validation geometry was modelled using three different EGSnrc libraries named ndgeometry, cylinders and genvelope. The materials density were taken from National Institute of Standards and Technology (NIST) as described in the report [8]. The *egs_collimated* source library was used to characterize the X-ray point source emitting a collimate beam towards the filter. The photon cross-section was defined as default and it includes the parameters of Rayleigh, Photoelectric, Pair Production as XCOM, and Bound Compton as Incoherent scattering. A number of 2×10^6 histories was used to have a uncertainties less than 1The photon fluence was also calculated using the EGSnr *egs_kerma* user code [10]. It returns the air kerma parameter in the volume defined by one or more geometric regions. The new user code was incorporated into the exercise as an alternative to compare the results to the cavity user code. New simulations were performed using same scheme as described in Figure 1, but replacing the scoring plane by an air sphere of 10 mm diameter and modeled using *egs_spheres* geometry. The following settings parameters,cross-sections,transport parameters, histories and uncertainties showed in Table 2 were kept the same and the forced detection (FD) variance reduction technique was used. The *egs_kerma* user code returns the normalized values of photon fluence

Table 3: Comparison of AK ratio coefficients obtained for the EGSnrc, MCNPX and TG-195.

					(Δ%)	
	Energy/Spectrum	**EGSnrc**	**MCNPX**	**TG-195 (average)**	**EGSnrc/TG**	**MCNPX/TG**
R1	30 keV	0.501	0.500	0.500	0.2	0.0
	100 keV	0.499	0.500	0.499	0.0	0.2
	30 kVp	0.500	0.502	0.500	0.0	0.4
	100 kVp	0.500	0.500	0.500	0.0	0.0
R2	30 keV	0.251	0.250	0.250	0.4	0.0
	100 keV	0.250	0.250	0.249	0.4	0.4
	30 kVp	0.250	0.252	0.250	0.0	0.8
	100 kVp	0.250	0.250	0.250	0.0	0.0
R3	30 keV	0.501	0.500	0.500	0.2	0.0
	100 keV	0.500	0.500	0.499	0.2	0.2
	30 kVp	0.500	0.502	0.500	0.0	0.4
	100 kVp	0.500	0.500	0.500	0.0	0.0
R4	30 keV	0.251	0.250	0.250	0.4	0.0
	100 keV	0.250	0.250	0.249	0.4	0.4
	30 kVp	0.250	0.252	0.250	0.0	0.8
	100 kVp	0.250	0.250	0.250	0.0	0.0

in units of cm^2 If the universe is filled with air material only scattered photons are considered. Thus, to calculate the non-scattered photons it must be considered vacuum rather than air which it is a slightly different from cavity which gives the option to choose the scattered and non-scattered photons. The simulation time for *egs_kerma* obtained was slightly different compared to *egs_kerma* and cavity, say, 0.012 hours and uncertainties less than 1 % were also obtained.

2.3. MCNPX

The Monte Carlo N-Particle Transport Code eXtended (MCNPX) code version 2.7 is a computational MC code that allows the modelling and simulating several and different radiation particles and electromagnetic waves. The ionization radiation transport through matter is made in a 3D arbitrary geometry [11]-[13]. The X-ray monoenergetic sources of 30 and 100 keV and two different spectra of 30 and 100 kVp were used in the validation simulations. The X-ray source emitting a characteristic X-ray beam was collimated in a conical geometry towards the scoring plane (or detector) placed at 1000 mm from the source. A semi-angle θ parameter was defined to have, in the direction of the z-axis, the emitting particles in a 10 mm field size in the scoring plane. The monoenergetic and polyenergetic X-ray beams were configured as described in the TG-195 exercise "Case 1" [7]. The tally card to score the planar fluence at the scoring plane used was the Tally F5 provided by MCNPX [11]-[13]. The detector has a 5 mm radius and it was placed at 1000 mm from the source. The simulations were performed in Orion cluster with 37 AMD Phenom (tm) II X6 1100T machines clocked at 3.3 GHz and 16 GB of memory, for a total of 222 cores. A number of particles adopted in the simulations were in an average of 5×10^8 number of started particles. An ideal nps can be achieved if the 10 statistical parameters and tested in the simulations with MCNPX are satisfied [11].

3. Results and Discussions

Table 3 shows the AK ratios results and it's deviations (Δ%) calculated using the EGSnrc cavity and MCNPX MC codes. The AK ratio coefficients were calculated using the Equations 2, 3, 4 and 5. These are the results obtained for the photon sources of 30 and 100 keV and two X-ray spectra of 30 kVp Molybdenum/Molybdenum (Mo/Mo) and 100 kVp Tungsten/Aluminum (W/Al) target/filter combinations. The results were then compared to the results published

Table 4: Comparison of AK ratio coefficients between the cavity and *egs_kerma* user codes on EGSnrc.

	Energy/Spectrum	Cavity	*egs_kerma*	Δ%
R3	30 keV	0.501	0.501	0.0
	100 keV	0.500	0.500	0.0
	30 kVp	0.500	0.500	0.0
	100 kVp	0.500	0.500	0.0
R4	30 keV	0.251	0.251	0.0
	100 keV	0.250	0.250	0.0
	30 kVp	0.250	0.250	0.0
	100 kVp	0.250	0.250	0.0

in the TG-195. The AK ratios R_1 and R_2 are the results obtained for the primary photon energies. Whereas the ratios R_3 and R_4 are the primary and the scattering photons summed. The deviation (Δ%) parameters are the results of the comparison between EGSnrc/MCNPX TG-195 report values. As it can be seeing in Table 3 the deviations are less than 1% for all results, saying maximum of 0.4% and 0.8% for EGS and MCNPX, respectively.

3.1. Validation *egs_kerma*

A new alternative to simulate the fluence of particles was added to the list of user codes of the EGSnrc MC code in 2019, called *egs_kerma*. Table 4 shows the AK ratio coefficients calculated from the simulations performed using the EGSnrc cavity and *egs_kerma* user codes. The uncertainties for both user codes were less than 1%. Therefore, the deviations (Δ%) obtained are 0% which match the results exactly the same for both volumetric and scoring plane considering the same diameter and for the different EGSnrc user codes.

4. Conclusion

The exercise "Case 1" of the American Association of Physics in Medicine (AAPM) - Task Group 195 (TG 195) named "Monte Carlo Reference Data Sets for Imaging Research" was modelled and simulated. The Air Kerma ratio values were calculated with EGSnrc and MCNPX MC codes and compared to the values published by the report AAPM TG-195. Differences less than 1 % were found when compared among the results. The intercomparison between the results obtained for the two MC codes was within the expected for the half and quarter value layers ratio calculated parameters. It was also incorporated in this exercise the newly *egs_kerma* user code of the EGSnrc. The main goal is to validate it by calculating the Air Kerma ratio parameters and comparing them to the cavity user code. The results obtained using the *egs_kerma* user code match exactly to the cavity. One difference between the user codes is the manner of modelling the detector surface, by using the new *egs_kerma* user code a sphere is needed, and it is the only difference seeing after all.

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Authorship contribution

L F Araújo (performed and led the simulations in the MCNPX code, discussion results), C V G Ferreira (performed simulations in the EGSnrc code, discussion results), F S G Silva performed simulations in the EGSnrc code, discussion results), F S G Silva (performed simulations in MCNPX code, discussion results), L Paixão (led the simulations performed in EGSnrc code, discussion results and reviewed the text) and T C F Fonseca (discussion results and textual review).

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Conflict of interest

This article has no conflict of interest and the authors have non-financial interests to disclose.

Declaration

This research has been conducted ethically, reporting of those involved in this article.

Similarity Index

I hereby confirm that there is no similarity index in abstract and conclusion while overall is less than 10% where individual source contribution is 2% or less than it.

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