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Simulation and Comparison of X-Ray Spectra in Diagnostic Radiography by IPEM 78, SpekPy, Xpecgen, SPEKTR 3.0, and EGSnrc Monte Carlo

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Abstract

This study presents the simulation results of the X-ray spectra of the general diagnostic radiography unit by using five computer codes.

The general diagnostic machine was assessed by quality assurance testing. The Half-Value Layer (HVL), mean energy (E_{mean}), and Air kerma per mAs (K_{air}/mAs) have been measured and compared with those obtained from five computer codes. The heel effect and target material composition were investigated. The IPEM report No.78 was used as a reference to compare with other computer codes.

The HVL, E_{mean}, K_{air}/mAs, and spectra were caused by five computer codes and the measurements showed that all have good agreement with the IPEM report No.78 and IEC 60601-1-3. The percentage differences (Diff, %) for HVL comparison vary between 1,16 to 3,71% for 70kVp, 0,64 to 3,61% for 80kVp, 0,11 to 3,13% for 90kVp. The Diff, % in E_{mean} comparison vary between 0,24 to 8,95% for 70kVp, 0,07 to 6,29% for 80kVp, 0,08 to 7,0% for 90kVp. The Diff, % in K_{air}/mAs comparison vary between 2,60 to 8,12% for 70kVp, 1,70 to 7,90% for 80kVp, 2,40 to 7,84% for 90kVp. For the anode heel effect, K_{air}/mAs is higher towards the cathode side and lower towards the anode side, and the difference is lower when aluminium filters are added.

The X-ray spectrum obtained by SpekPy is in the best agreement with IPEM report No.78 while Xpecgen, Spektr 3.0, EGSnrc MC show a significantly lower K-peaks intensity for 80 and 90kVp. The comparative assessment showed that the HVL, E_{mean} and K_{air}/mAs were well-matched between the five codes and physical measurements.

Keywords: IPEM report No.78; SpekPy; Xpecgen; Spektr 3.0; EGSnrc Monte Carlo

Introduction

General radiography is an important, quick, and painless diagnostic tool in medical imaging to spot problems in the body's internal structures. X-ray machine is widely used in hospitals, and clinics and has become an indispensable medical diagnostic method. We now have a better understanding of the risks associated with X-ray radiation and have developed protocols to minimize significantly unnecessary exposure. The accurate knowledge of the X-ray spectrum provides useful information for physicists, designers, manufacturers, radiation dosimetry, and doctors to minimize the radiation dose and improve image quality. Thus, experimental measurements are very complex and time-consuming, other methods of predicting X-ray spectra have been developed to generate X-ray spectra from tungsten targets. These methods are divided into three categories: Empirical [1-5], semi-empirical models [6-10], and MC simulations [11-15]. The MC method is a sophisticated, precise computational tool that can characterize the spectra of newly developed target material compositions, complex geometrical configurations, and contributions of secondary particles, which are mostly empirical and semi-empirical models that currently can't be performed accurately.

In this paper, we use five different computer codes (IPEM 78, SpekPy, Xpecgen, Spektr 3.0, and EGSnrc MC to simulate the diagnostic radiography X-ray tube at 70, 80 and 90kVp to generate X-ray spectra. The HVL, E_{mean}, and K_{air}/mAs have been measured, and compared with those from the simulated. The simulated X-ray spectra were compared with those from IPEM report No.78 [Institute of Physics and Engineering in Medicine (IPEM)] [16]. In addition, the anode heel effect and target material composition were evaluated. The HVL, E_{mean}, spectra, and K_{air}/mAs were caused by five computer codes and the measurements showed that all have good agreement with the IPEM

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report No.78 and IEC 60601-1-3 requirements [17].

Materials and Methods

Computer codes

EGSnrc – Electron Gamma Shower from National Research Council Canada [14] - a software toolkit released in 2020, utilities to build MC simulation of ionizing radiation transport (photons, electrons, positrons) through matter and complex geometries with energies from 1 keV to 10 GeV. In this study, the simulations were divided into two steps using the software included in the default installation package of EGSnrc: First, the X-ray machine was simulated using the BEAMnrc [18] to obtain spectrum at three kVps. The measurements and simulations were performed with a TXR full wave radiography X-ray machine, tube model E 7239 GX with serial number 14C 413 (Toshiba/Japan, marketed in 2014), with an anode diameter of 74 mm, an angle is 16 degrees, the target was built as rhenium-tungsten (90%W/10%Re) faced molybdenum, and 2.5 mmAl equivalent filter (inherent filtration of 0.9 mmAl and an additional filter of 1.6 mmAl). The target was encased in a vacuum with 0.20 cm thick Pyrex glass. The X-ray tube housing is 0.20 cm thick of lead, below is the collimator with four lead shutters 0.20 cm thick, along with a light and mirror (1 mmAl equivalent) to determine the light and radiation fields. The voltage ripple is less than 2%, but not considered in this simulation. A geometric schematic of the X-ray tube and collimator for EGSnrc simulation was shown in Figure 1 (not to scale).

The simulations were made with Ncase = 1E8 histories, this was enough to achieve the statistical accuracy, electron and photon energy cut-off: 0.512 MeV and 0.001 MeV, ISOURC = 10 with the pencil electron beam of 0.13 cm radius incident from the side. The .pegs4dat file that contains cross-section information of all needed media can be done by using egs gui. The phase-space files were calculated at a distance of 75 cm from the center of the target.

The HVL, E_{mean}, and spectra of each kVp were obtained using egs cavity [19]. The phase-space files obtained from BEAMnrc were used as input to run the egs_cavity user code.

The calculations were made with Ncase = 1E6 histories, photon splitting = 1000, electron and photon energy cut-off: 0.512 MeV and 0.001 MeV. The energy bin interval is 0.5 keV. The HVL values were obtained by using the two-point method [20]. The target materials were evaluated with various compositions of rhenium (0%Re, 5%Re, 10%Re, 15%Re, 20%Re, and 30%Re). Table 1 was shown the materials and inputs used to simulate this model. Summary of computer codes used for generation of X-ray spectra were shown in Table 2.

SpekPy – a Python programming language toolkit to generate X-ray spectra from tungsten, molybdenum, and rhodium targets [21]. The fluence, K_{air}, E_{mean}, E_{eff}, first and second HVL values (in mmAl and mmCu), and homogeneity coefficient can be calculated from the spectrum. The keywords arguments in SpekPy were: targ = W (anode material), kvp = 70/80/90 (tube voltages in kV), th = 16 (anode angle in degree), dk = 0.5 (bin width in keV), physics = “default” (name of the physics mode), mu data source = “pene” (linear attenuation data), char = True (whether the characteristic portion of spectrum is retained), brem = “True” (whether the bremsstrahlung portion of spectrum is retained), mas = 10 (The exposure setting for the file spectrum), z, x, y = 75, -5, 5 (point of interest in cm), obli = True (whether path-length through extrinsic filtration varies with x, y). SpekPy also can create a new material filter using weights with keywords: material density (g/cm^3) and material composition (atomic number, weight). The output spectrum was exported to .spk files. In this study, SpekPy was used for evaluating the anode heel effect at 90kVp with and without aluminium filters.

Table 1: Materials and density in g/cm^3 of EGSnrc MC simulation.

Material	Element	Density, g/cm^3
Anode	90%W/10%Re	19,427
Pyrex glass	B, O, Na, Al, Si, K	2.23
Air	C, N, O, Ar	$1,2048 \times 10^{-3}$
Lead shielding/collimator shutters	Pb	11.35
Filter	Al	2.7
Anode axis	Mo	10.28

Xpecgen – a Python package to calculate X-ray spectra generated in tungsten anode using the model from [22] at 100 cm from the focal spot. The parameters used for calculation are given: E0 = 70/80/90 (Electron kinetic energy in keV), theta = 16 (X-ray emission angle in degrees, e_min = 3 (minimum kinetic energy to calculate in the spectrum in keV), num_e = 120 (Number of points to calculate in the spectrum), epsrel = 0.5 (The tolerance parameter used in numeric integration). The output files are available in formats .csv, .xlsx, and .pkl.

Spektr 3.0 [23] – a MATLAB [24] toolkit for calculation of X-ray spectra, beam quality, HVL K_{air}, and fluence per unit exposure from 1 keV to 150 keV in 1 keV energy bins using Tungsten Anode Spectral Model using Interpolating Cubic Splines (TASMICS) algorithm [25] at 100 cm from the focal spot. The main modules of this toolkit are: spektr.m - start graphical user interface, spektrAirKerma.m - calculate K_{air} for the inputted spectrum, spektrFluencePerAirKerma.m - generates the fluence per Air Kerma, spektrExposure.m generates the exposure, spektrHVLn.m - calculates the n’th HVL (n - number of the half value layers to calculate), spektrMeanEnergy.m - function returns the mean energy of the X-ray spectra, spektrSpectrum.m - function will generate an X-ray spectrum at the specified potential (of the generator) that is set to a constant 1 mAs.

IPEM report No.78 – a software provides spectra from a tungsten target with an anode angle of 6 to 22 degrees at tube voltages ranging 30 kV to 150 kV and spectra from molybdenum and rhodium with an anode angle of 9 to 23 degrees at tube voltages ranging 25 kV to 32kV. The additional filter can be made out of various materials, energy bin in all spectra was provided 0.5 keV. Due to its popularity and widespread availability in the radiological physics field, the IPEM report No.78 was used as a reference to compare with other computer codes.

All simulations were performed in a computer with Intel Core i5-4200U CPU 1, 60 GHz. The time of each simulation was about a minute to 7 h. All output data files obtained from those computer codes were summarized, analyzed, and plotted in Mathematica software [26].

Quality Assurance (QA) using non-invasive Accu-Gold+ Touch Pro diagnostic X-ray system

The X-ray general diagnostics machine was assessed by testing parameters like reproducibility of kVp, dose output, and time exposure; accuracy of kVp, time exposure; mAs linearity, and HVL. All tested parameters must be matched to the national or/and international tolerance limits.

Table 2: Summary of computer codes used for generation of X-ray spectra.

Computer codes	Catalog	Base on model	Electron model	Bremsstrahlung model	Focal to Detector distance, cm
EGSnrc	MC simulation	MC	PRESTA-II	NIST data	75
SpekPy	Semiempirical	SpekCalc	Diffusion approximation	UNI	75
Xpecgen	Semiempirical	Birch and Marshall model	Explicit	UNI	100
		(target pure W)			
Spektr 3.0	Empirical	TASMICS model	MCNPX	MCNPX	100
IPEM 78	Semiempirical	Birch and Marshal model	Thomson-Whiddington	UNI	75
		(90/10 W/Re)			

Table 3: The resulting test of QA for the general diagnostic X-ray machine.

No	Parameters	Selected kVp	Error, %	Baseline	Status
1	kVp accuracy	70	-1.29	less than ± 10% or	pass
		80	-0.54	less than ± 10 kV	pass
		90	0.90		pass
2	kVp reproducibility	70	0.00	less than ± 5%	pass
		80	0.04		pass
		90	0.07		pass
3	Exposure time reproducibility	70	0.00	less than ± 10%	pass
		80	0.07		pass
		90	0.07		pass
4	Exposure time accuracy	70	-0.47	less than ± 20 % for times <100 ms	pass
		80	-0.54		pass
		90	-0.44		pass
5	Reproducibility of radiation output	70	0.11	less than ± 5%	pass
		80	0.09		pass
		90	0.07		pass
6	Coefficient of linearity	70	0.01	less than 0.1	pass
7	Radiation output linearity		1.44	less than ± 20%	pass

The physical measurements were performed using a calibrated Accu-Gold+ Touch Pro (AGT-P-AG, serial number 55-2036) with solid-state Accu-Gold Multi-Sensor (AGMS-DM, serial number 431483). AGMS-DM sensor enables the measurement of dose, dose/mAs, dose/pulse, dose rate, HVL, kVp, exposure time, pulse count with kVp ranging 20 to 160 (uncertainty 2%), exposure time ranging 1 min to 300 s (uncertainty 0.1%), HVL ranging 0.16 mmAL to 13.5 mmAL with W anode (uncertainty 10%), dose rate ranging 80 nGy to 100 Gy (uncertainty 5%). Routine calibration of the QA system is required annually, traceable to the Secondary Standard Dosimetry Laboratory, Institute for Nuclear Science and Technology, Vietnam. The sensor was placed 75 cm from the focal spot, radiation field of 10 × 10 cm^2.

The QA test was taken 3 times for each kVp. For estimation E_{mean}, the mass attenuation coefficients (μ/ρ) were calculated from physical measurements of HVL by using the equation: $\mu = \ln 2/HVL$ and aluminium density $\rho = 2.7\ g/cm^3$. The National Institute of Standards and Technology (NIST) data table [27] was used for extrapolation deposition X-ray energy by using the NonLinearModelFit model of the Mathematica to link the points, then the E_{mean} evaluated the fitted function at each HVL value. The Plot function was used to visualize the fitted function with the data. The ratio of intensity K-peaks obtained from computer codes to IPEM report No.78 was calculated by using the following equation: $R = I_x/I_{IPEM}$ where Ix: intensity of K-peaks obtained from EGSnrc MC, Spektr 3.0, SpekPy, and Xpecgen codes at 80 and 90 kVp. I_{IPEM}: Intensity of K-peaks obtained from IPEM 78 code.

Results

The study of QA consists of reproducibility of kVp, dose output, and time exposure; accuracy of KVp, time exposure; mAs linearity, and HVL, was given in Table 3. The comparisons of simulated X-ray spectra for various tube voltages were shown in Figures 2-4. The comparisons of HVL, E_{mean}, K_{air}/mAs, and K-peaks energies and their ratio intensity of X-ray were shown in Tables 4-7. The anode heel effect was shown in Figure 5, 6. The assessment of various target compositions was illustrated in Figure 7. The fitted function used to estimate E_{mean} from physical measurements of the HVL was shown in Figure 8. The Coefficient of Linearity (CoL) was shown in Figure 9. The minimum requirements of the first HVL in mmAL established IEC-60601-1-3 were shown in Figure 10.

Discussion

QA study

The QA for the X-ray machine was shown good results for all tested parameters within the limit of [28,29]. As shown in Table 3, the accuracy of kVp gave a maximum % error of less than -1.29% which is lower than the limit (less than -10%). Maximum exposure

Table 4: Evaluation of five computer codes for HVL estimations for various tube voltages.

Computer codes	70 kVp		80 kVp		90 kVp	
	HVL, mmAl	Diff, %	HVL, mmAl	Diff, %	HVL, mmAl	Diff, %
IPEM report No.78	2.84	-	3.25	-	3.68	-
Spektr 3.0	2.93	3.34	3.33	2.58	3.73	1.50
SpekPy	2.80	1.16	3.18	2.18	3.57	3.13
Xpecgen	2.90	2.13	3.28	0.86	3.67	0.11
EGSnrc MC	2.94	3.71	3.37	3.61	3.76	2.30
Measured	2.88	1.50	3.27	0.64	3.62	1.62
IEC 60601-1-3	>2.5		>2.9		>3.2	

Table 5: Comparison of the E_{mean} at various tube voltages.

Computer codes	70 kVp		80 kVp		90 kVp	
	E_{mean}, keV	Diff, %	E_{mean}, keV	Diff, %	E_{mean}, keV	Diff, %
IPEM report No.78	40.80	-	44.50	-	47.80	-
Spektr 3.0	40.99	0.47	44.53	0.07	47.76	0.08
SpekPy	40.90	0.24	44.46	0.09	47.73	0.16
Xpecgen	42.98	5.21	47.05	5.56	50.89	6.27
EGSnrc MC	38.54	5.69	42.05	5.66	44.57	7.00
Measured	44.62	8.95	47.39	6.29	48.47	1.40

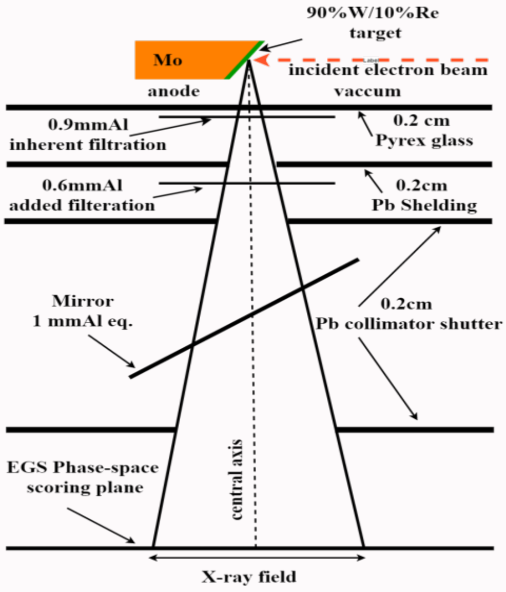

Figure 1: Geometric schematic of the X-ray tube and collimator for EGSnrc simulation.

time accuracy equals -0.54% which is lower than the limit (less than -20% for time less than 100 ms). Reproducibility of kVp varies from 0% to 0.07% lower than the limit (less than -5%). The reproducibility of radiation output varies from 0.07% to 0.11% lower than the limit (less than -5%). Reproducibility of exposure time varies from 0% to 0.07% lower than the limit (less than -10%). Milliampere-second (mAs) linearity at 70kVp equals 1.44% lower than the limit (less than -20%). The CoL at 70kVp equals 0.01 which does not exceed the limit (less than 0.1).

Simulation of X-ray spectra in diagnostic radiography

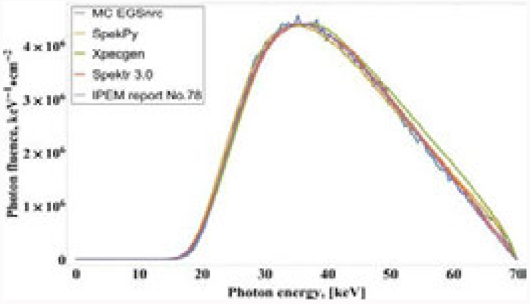

Figure 2: Comparison of the simulated X-ray spectra for 70kVp produced by five computer codes.

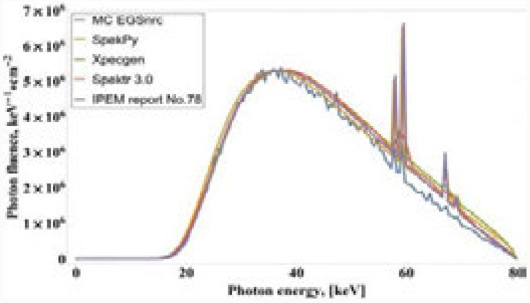

Figure 3: Comparison of the simulated X-ray spectra for 80kVp produced by five computer codes.

Figures 2-4 show that, five computer codes are all very good at predicting the spectrum of general X-ray machine used in diagnostic radiography. On the other hand, it is possible to be seen that, a slight difference in the characteristics of K-peaks ($K_{\alpha1}$, $K_{\alpha2}$, $K_{\beta1}$, $K_{\beta2}$). The spectrum of IPEM report No.78 and SpekPy codes have very good congruence and clearly distinguish K-peaks, while Spektr 3.0 and Xpecgen have a superposition of $K_{\alpha1}$ and $K_{\alpha2}$, $K_{\beta1}$ and $K_{\beta2}$ peaks. EGSnrc MC shows the "hardest" spectrum of all-over codes. The energy of K-peaks also varies slightly between computer codes (Table 7). The ratio of the peak intensity to IPEM report No. 78 shows that:

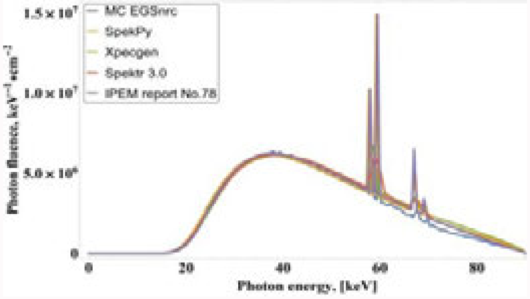

Figure 4: Comparison of the simulated X-ray spectra for 90kVp produced by five computer codes.

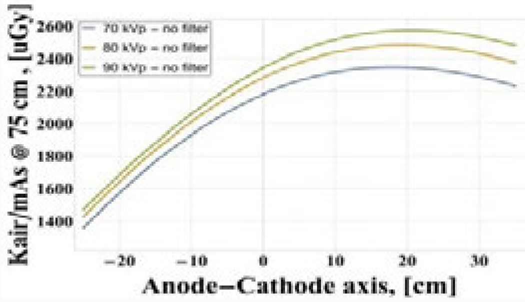

Figure 5: SpekPy simulated heel effect for anode without an aluminum filter at tube voltages 70kVp, 80kVp, and 90kVp.

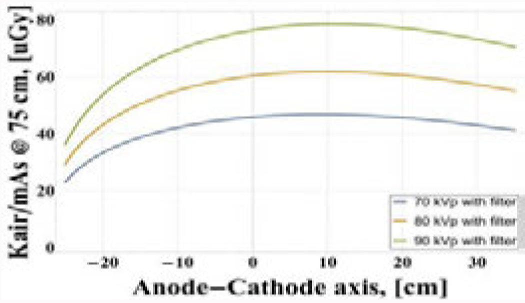

Figure 6: SpekPy simulated heel effect for anode with an aluminum filter at tube voltages 70kVp, 80kVp, and 90kVp.

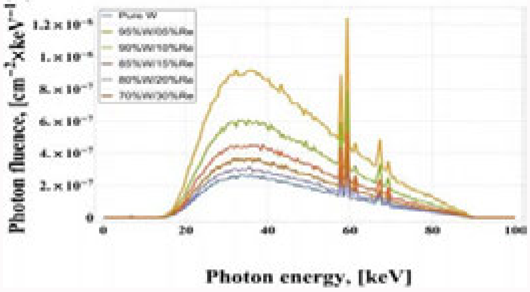

Figure 7: EGSnrc MC simulated spectra for various target compositions at tube voltage 90kVp.

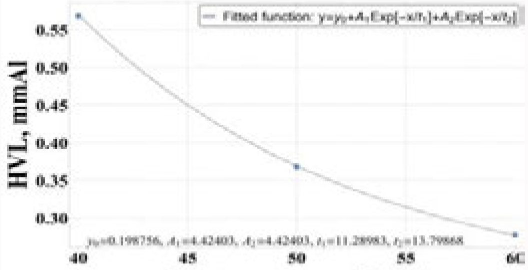

Figure 8: The fitted function was used to estimate E_{mean} from physical measurements of the HVL.

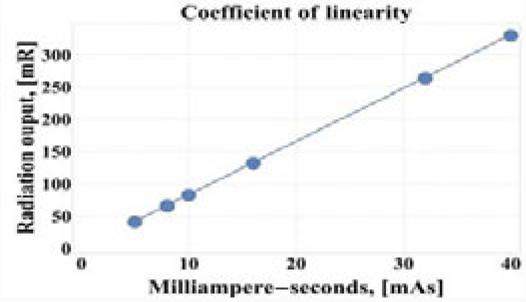

Figure 9: CoL calculated at 70kVp.

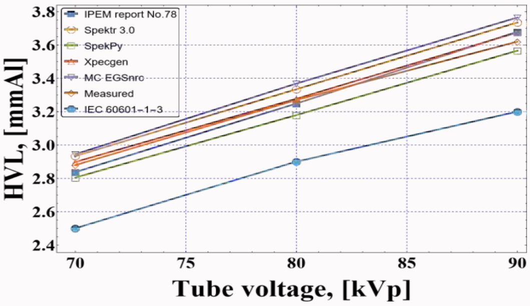

Figure 10: The minimum requirements of the first HVL in mmAL established IEC-60601-1-3.

SpekPy has the best agreement with the ratio varying from 0.85 to 1.02 at 80 kVp and from 0.77 to 1.00 at 90 kVp. The intensity of K-peaks X-ray production by Xpecgen, Spektr 3.0 and EGSnrc MC codes is significantly lower than IPEM report No. 78 with the ratio varying from 0.39 to 0.84 (Table 7). The discrepancy of the simulated X-ray spectrum among five computer codes can be explained by the difference in the fitting model and the difference in electron and bremsstrahlung models as shown in Table 2. On the other hand, IPEM report No. 78 and EGSnrc MC use a W/Re target with 10% Re while SpekPy, Xpecgen, and Spectr 3.0 use a pure W target should be taken into account when comparing this difference.

Comparisons of the HVL, E_{mean}, and K_{air}/mAs at various tube voltages

Table 4 compares the HVL for various tube voltages of physical experiments and simulated using five computer codes. The percentage differences vary between 1.16% to 3.71% for 70 kVp, 0.64% to 3.61% for 80 kVp, and 0.11% to 3.13% for 90 kVp. The percentage differences of SpekPy increase while other computer codes decrease with increasing tube voltage. All simulated and physical measurements of HVL for various kVp satisfied the minimum requirements of IEC-60601-1-3. Table 5 compares the E_{mean} for various tube voltages of physical experiments and simulated using five computer codes. The percentage differences vary between 0.24% to 8.95% for 70 kVp, 0.07% to 6.29% for 80 kVp, and 0.08% to 7.00% for 90 kVp. Table 6 compares the K_{air}/mAs for various tube voltages of physical experiments and simulated

Table 6: Comparison of K_{air}/mAs (at 100 cm for Spektr 3.0 and Xpecgen codes).

Computer codes	70 kVp		80 kVp		90 kVp	
	K_{air}/mAs, Gy	Diff, %	K_{air}/mAs, Gy	Diff, %	K_{air}/mAs, Gy	Diff, %
IPEM report No.78	101.60	-	132.90	-	167.00	-
Spektr 3.0	51.86	8.12	70.67	5.62	98.73	4.97
SpekPy	104.28	2.6	135.23	1.74	163.03	2.40
Xpecgen	51.71	8.41	69.69	7.01	97.77	7.84
EGSnrc MC	98.76	2.83	130.32	1.96	163.12	2.35
Measured	95.40	6.29	122.74	7.95	155.15	7.36

Table 7: Evaluation of X-ray characteristics K-peaks at 80kVp and 90kVp.

kVp	K-peaks	Literature	IPEM report No.78	Spektr 3.0	SpekPy	Xpecgen	EGSnrc MC
			Peak, keV	Peak, keV	Peak, keV	Peak, keV	Peak, keV
80	$K_{\alpha2}$	57.98	58	-	57.75	-	57.75
	$K_{\alpha1}$	59.32	59.5	59	59.25	58.72	59.25
	$K_{\beta1}$	67.24	67	67	67.25	67.23	64.25
	$K_{\beta2}$	69.10	69	-	69.25	-	67.25
90	$K\alpha_2$	57.98	58	-	57.75	-	58.25
	$K\alpha_1$	59.32	59.5	59	59.25	58.54	59.75
	$K_{\beta1}$	67.24	67	67	67.25	67.27	67.75
	$K_{\beta2}$	69.10	69	-	69.25	-	69.75

Table 8: Differences in K_{air}/mAs at 100 cm from focal spot obtained by SpekPy at various kVp.

kVp	Difference in K_{air}/mAs, %	
	with aluminium filter	without aluminium filter
70	39.46	31.31
80	40.72	33.77
90	41.75	35.96

using five computer codes. The percentage differences vary between 2.60% to 8.12% for 70 kVp, 1.70% to 7.90% for 80 kVp, and 2.40% to 7.84% for 90 kVp.

Assessment of anode heel effect and anode composition in diagnostic radiography

Figure 5 illustrates the anode heel effect at various kVp. Differences in K_{air}/mAs from -20 cm anode side to 20 cm cathode side of the central axis with and without aluminium filer were shown in Table 8. It can be seen that the difference in K_{air}/mAs of the diagnostic radiography increases by increasing the kVp. Otherwise, the difference is lower when aluminium filters are added, which enables the diagnostic imaging to achieve uniformity in radiation intensity. This is one of the important factors to achieve the quality of images and diagnostic accuracy. One of the factors affecting the X-ray emission efficiency of target materials is the atomic number. In general, diagnostic radiography, the target material is usually rhenium-tungsten faced molybdenum in different proportions depending on the manufacturer. In this study, we present the results of the simulation of the X-ray spectrum with target materials with %W/%Re ratios of 100W/0Re, 95W/05Re, 90W/10Re, 85W/15Re, 80W/20Re, and 70W/30Re. Figure 6 shows the EGSnrc MC simulated spectra for various target compositions at 90 kVp. The total fluence over the spectrum was normalized to unity. It is clearly seen that the total fluence is highest at 95%W/5%Re and then gradually decreases with %Re of 10, 15, 30, and 20%. Pure W target has the lowest total fluence. Although the target with 95%W/05%Re has the highest efficiency, the X-ray spectra produce more low-energy photons, which affects the contrast of the image and causes an increase in the patient exposure dose. Therefore, this study provides useful results when designing targets to ensure a balance between minimizing patient exposure dose and X-ray image quality.

Conclusion

In this study, five computer codes were employed to simulate the X-ray spectrum and compared the X-ray spectrum between these five codes. The comparison results show that the X-ray spectrum obtained by SpekPy is in the best agreement with IPEM report No. 78 while Xpecgen, Spektr 3.0 and EGSnrc MC show a significant difference in K-peaks intensity. The intensity of K-peaks in IPEM report No. 78 and SpekPy are significantly higher than Xpecgen, Spektr 3.0 and EGSnrc MC for 80 and 90 kVp. The comparative assessment showed that the HVL, E_{mean} and K_{air}/mAs were well-matched between the five codes and physical measurements. The HVL obtained from the simulations satisfied the minimum requirements of IEC-60601-1-3. The anode heel effect and target material composition were also evaluated by using SpekPy and EGSnrc MC codes, respectively. Empirical and semi-empirical codes can quickly provide calculation results, just under a minute, but these models have the limitation that they cannot be flexibly applied to any target/filter materials and geometry configurations. The MC simulation is time-consuming but the results provide more detailed information's about the electron interaction to target/filter combinations with any material composition. This is useful when designing new target materials as well as achieving the image quality requirements in diagnostics radiography.

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