SpekCalc: a program to calculate photon spectra from tungsten anode x-ray tubes

2009 Phys. Med. Biol. 54 N433

(http://iopscience.iop.org/0031-9155/54/19/N01)

IOP PUBLISHING PHYSICS IN MEDICINE AND BIOLOGY

Phys. Med. Biol. **54** (2009) N433–N438 doi:10.1088/0031-9155/54/19/N01

NOTE

SpekCalc: a program to calculate photon spectra from tungsten anode x-ray tubes

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Received 3 June 2009, in final form 10 August 2009
Published 1 September 2009
Online at stacks.iop.org/PMB/54/N433

Abstract

A software program, *SpekCalc*, is presented for the calculation of x-ray spectra from tungsten anode x-ray tubes. *SpekCalc* was designed primarily for use in a medical physics context, for both research and education purposes, but may also be of interest to those working with x-ray tubes in industry. Noteworthy is the particularly wide range of tube potentials (40–300 kVp) and anode angles (recommended: 6–30°) that can be modelled: the program is therefore potentially of use to those working in superficial/orthovoltage radiotherapy, as well as diagnostic radiology. The utility is free to download and is based on a deterministic model of x-ray spectrum generation (Poludniowski 2007 *Med. Phys.* **34** 2175). Filtration can be applied for seven materials (air, water, Be, Al, Cu, Sn and W). In this note *SpekCalc* is described and illustrative examples are shown. Predictions are compared to those of a state-of-the-art Monte Carlo code (BEAMnrc) and, where possible, to an alternative, widely-used, spectrum calculation program (IPEM78).

1. Introduction

The x-ray tube, although first developed in the late 1800s, remains today a vital piece of equipment in hospitals, industry and research. As such there is a need to efficiently predict x-ray emission spectra from a given tube, as well as beam qualifiers such as the first

half-value-layer (HVL_1) and the second half-value-layer (HVL_2). We present a free-to-download program, *SpekCalc*, for simulating x-ray spectra emitted from thick-target tungsten anode x-ray tubes. *SpekCalc* was primarily developed for research and education in medical physics, although applications in other fields of radiation physics are possible. The range of tube potentials covered is such that, within medical physics, the program is of interest to those working in superficial and orthovoltage radiotherapy as well as in diagnostic radiology. In this note, we describe the software, briefly explain the underlying model and provide some examples. The *SpekCalc* model relies on deterministic equations for bremsstrahlung productions, combined with numerically pre-calculated electron distributions and has been described elsewhere (Poludniowski and Evans 2007, Poludniowski 2007). The primary objective of this note is to introduce the *SpekCalc* utility, not to rigorously evaluate it against data. For the illustrative examples, we do, however, compare against calculations with a state-of-the-art Monte Carlo code (Rogers *et al* 2002) and to a commonly used software program (Cranley *et al* 1997) that is based on a simpler, semi-empirical, method.

2. Theoretical background

Within an x-ray tube, an electron beam is directed to a focal spot on a metal anode. As these electrons penetrate the target, they scatter from electrons and nuclei in the target, resulting in bremsstrahlung and, depending on their energies, characteristic emissions. These emissions produce the observed x-ray spectrum. Semi-empirical models of x-ray production treat the penetration and energy loss of the incident electron beam crudely (e.g. Birch and Marshall 1979). In contrast, state-of-the-art Monte Carlo codes, such as BEAMnrc (Rogers *et al* 2004), treat particle transport with great rigour. The theoretical approach underlying *SpekCalc* combines elements of the two approaches. The survival probabilities for an electron reaching certain depths within the target, and, the electron energy distributions at those depths, have been pre-calculated using BEAMnrc (Poludniowski and Evans 2007). The bremsstrahlung cross-section is treated using analytical theory, and the self-filtration within the anode is treated similarly to in semi-empirical approaches. The predictions of *SpekCalc* model have shown satisfactory agreement with experimentally measured spectra, where tested (Poludniowski 2007). Although calculated for pure tungsten anodes, the predictions are applicable to commonly used (tungsten-dominated) tungsten–rhenium alloys. We add the caveat that as the proportion of rhenium is increased, there are likely to be increasing discrepancies in the characteristic part of the spectrum.

The gold standard technique for x-ray tube calculations remains the Monte Carlo method. Historically, Monte Carlo calculations have suffered from long computation times. Yet, with modern computing power and the use of powerful variance reduction techniques, Monte Carlo approaches are becoming increasingly fast for this task, taking perhaps as little as a few minutes: see, for example, Verhaegen *et al* (1999), Mainegra-Hing and Kawrakow (2006) and Ali and Rogers (2007). Utilities such as *SpekCalc* still retain some advantages. Firstly, *SpekCalc* is computationally very fast (each calculation takes a few seconds). Secondly, the program and data are small (a single 6 MB executable and a few data files). Thirdly, and importantly, it quickly and conveniently provides information, such as HVLs, to the user. Alternative computer programs aimed at those working in diagnostic radiology *do* exist, but these have typically been empirically or semi-empirically based. An example of such a program is the Spectrum Processor of the Institute of Physics and Engineering in Medicine's Report 78 (IPEM78), available on a CD-ROM for a small fee, based on the three-decade old model of Birch and Marshall (1979). However, to our knowledge no such program, aside from *SpekCalc*, extends its predictions to orthovoltage x-ray beams.

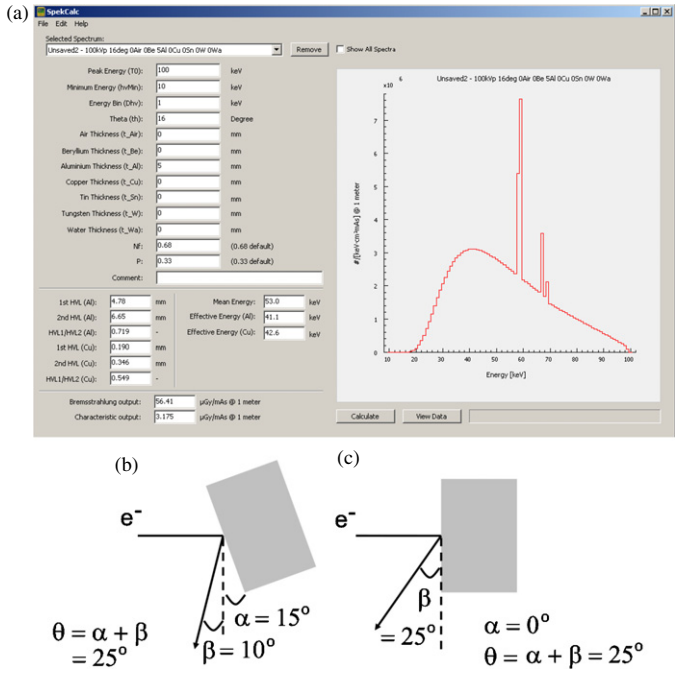

Figure 1. (a) Screenshot of the *SpekCalc* GUI, (b) illustration of angles α, β and θ for an inclined anode, and (c) illustration of angles α, β and θ for a perpendicular anode.

(This figure is in colour only in the electronic version)

3. The *SpekCalc* program

SpekCalc was created using REALbasic (REAL software, Inc.), and versions of the executable are available for both Windows and Mac O/S. The utility allows the user to calculate, display and save, in energy bins of user-defined width, the x-ray spectra emitted from tungsten anode x-ray tubes. A screenshot of the Graphical User Interface (GUI) is shown in figure 1(a). The user selects the electron energy in keV, the x-ray take-off angle and the amount of filtration. Following a click of the 'Calculate' button, a spectrum is presented within a few seconds. The anode take-off angle is defined to be θ. This parameter can be interpreted as the sum of the anode angle, α, and the off-axis escape angle, β. The geometry with respect to the anode is illustrated in the example of figure 1(b). Note that only the sum of α and β (i.e. θ) is significant, in the model, so that the situations of figures 1(b) and (c) will produce identical predictions. No restriction is set on the value of θ, but we recommend the user remains in the range: 6–30°. Several beam qualifiers are presented by the *SpekCalc* GUI: HVL_1 and HVL_2 in mm of both Al and Cu; the mean energy of the spectrum, E_{mean}, and the effective energy, E_{eff}, for Al and Cu, in keV. E_{mean} is defined as the mean beam energy averaged over the fluence spectrum. E_{eff} for Al (or Cu) is the energy of a monoenergetic beam that would produce the same HVL_1 value in Al (or Cu). Additionally, the estimated bremsstrahlung and characteristic contributions to the tube output ($\mu Gy/mAs$ @ 1m) are displayed. Filtration can be selected in mm, for 7 materials: Al, Cu, W, Sn, Be, water and air. This allows an exploration of the filtration effects of materials of differing atomic numbers. The model parameters 'Nf' and 'P' in the GUI take the default values of 0.68 and 0.33 (Poludniowski 2007). The former normalizes the overall fluence and

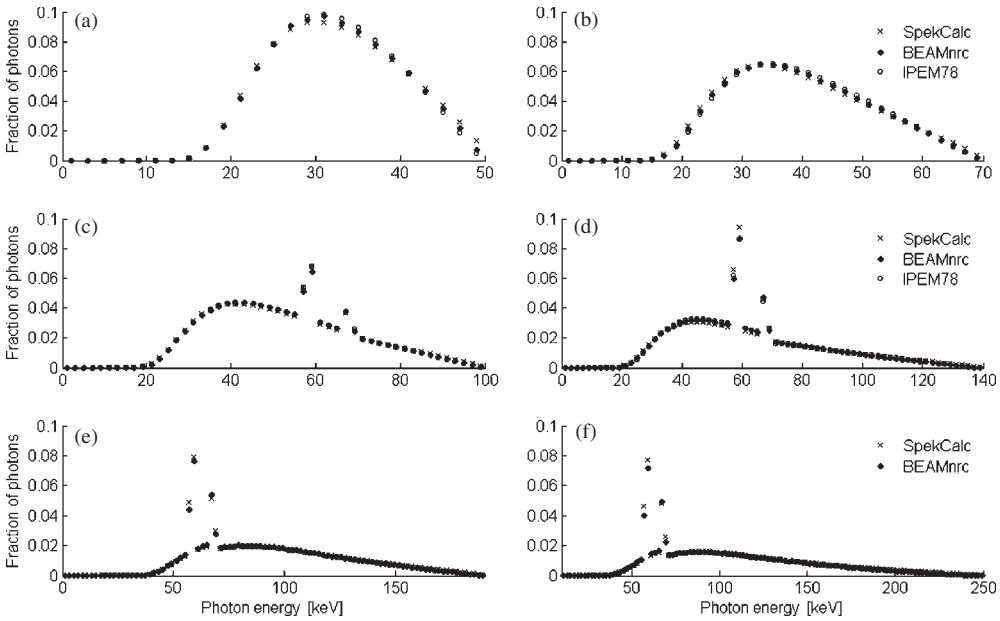

Figure 2. X-ray tube spectrum predictions for *SpekCalc*, IPEM78 and the BEAMnrc model: (a) 50 kV, (b) 70 kV, (c) 100 kV, (d) 140 kV, (e) 190 kV and (f) 250 kV. Note: IPEM78 predictions not available for (e) and (f).

can be used to match the output prediction to that of a particular tube, if desired. The latter is the ratio of the number characteristic x-rays produced via electron impact ionization to that generated by photoelectric absorption of bremsstrahlung; this ratio should not be changed without justification. The range of potentials that can be modelled is wide (40–300 kV) making the utility useful to both the diagnostic imaging and superficial/orthovoltage radiotherapy fields. It should be emphasized that, currently, *SpekCalc* does not provide predictions relevant to mammography, where different anode materials would have to be considered and the characteristic x-ray contributions modelled more comprehensively. Nor are the predictions of the program suitable for the modelling of transmission targets. Future releases may extend the domain of validity and capabilities of the program. *SpekCalc* may be downloaded from the following webpage: http://www.icr.ac.uk/research/research_sections/physics/3544.shtml.

4. Illustrative examples

To illustrate the predictions of *SpekCalc*, three x-ray tubes were simulated. The first was assumed to have a 10° anode angle and a filter of 2.5 mm of Al. Central-axis spectra were calculated for 50 and 70 kV tube potentials. The second tube was taken to have a 16° anode angle and 5.0 mm of Al filtration. Spectra were calculated for this tube at 100 and 140 kV potentials. For the final x-ray tube, a 24° anode angle was selected combined with 1.0 mm of Cu filtration, and spectra were calculated at potentials of 190 and 250 kV.

To demonstrate the accuracy of *SpekCalc*, the predictions of the utility were compared with those of the BEAMnrc Monte Carlo program. We note that the calculations of keV x-ray spectra with BEAMnrc have shown good agreement with experimental measurements (Mainegra-Hing and Kawrakow 2006). The 'Component Modules' in the BEAMnrc simulations consisted of

Table 1. X-ray beam qualifiers for the *SpekCalc*, IPEM78 and BEAMnrc models.

	kV	50	70	100	140		190	250	
BEAMnrc	HVL_1 (mm)	1.77	2.45	4.81	6.48	Al	1.36	1.87	Cu
	HVL_2 (mm)	2.33	3.52	6.62	8.92	Al	2.04	2.93	Cu
	E_{mean} (keV)	32.3	39.7	52.7	62.5		93.5	107.1	
	E_{eff} (keV)	27.3	30.9	41.2	48.0		90.6	105.0	
SpekCalc	HVL_1 (mm)	1.74	2.38	4.78	6.46	Al	1.39	1.93	Cu
	HVL_2 (mm)	2.32	3.46	6.65	8.97	Al	2.11	3.03	Cu
	E_{mean} (keV)	32.4	39.6	53.0	62.8		94.6	109.0	
	E_{eff} (keV)	27.1	30.6	41.1	47.9		91.5	106.6	
IPEM78	HVL_1 (mm)	1.83	2.59	4.91	6.70	Al			
	HVL_2 (mm)	2.38	3.66	6.69	9.03	Al			
	E_{mean} (keV)	32.5	40.1	52.9	62.9				
	E_{eff} (keV)	27.6	31.6	41.6	48.9				

an 'XTUBE' (the x-ray target) and a 'SLABS' (the filter). The cross-sections from the NIST database were selected. AE (inelastic collision threshold) and AP (photon production threshold) were set to 512 keV and 1 keV, respectively. ECUT (electron transport cutoff) and PCUT (photon transport cutoff) were set to 521 and 10 keV, respectively. Rayleigh scattering and bound Compton scattering were switched on, along with atomic relaxations and electron impact ionization. Directional bremsstrahlung-splitting was selected, with a splitting factor of 10^4, in the direction of the scoring region. This scoring region was a circle of 1.0 cm radius placed at 50 cm from the focus, at right angles to the incident electron beam. The photons in the resulting phase-space files were assigned into energy bins of width 2 keV. Simulations were performed for several 10^8 histories, to ensure negligible statistical uncertainties for each energy bin. HVLs were calculated deterministically from the BEAMnrc spectra, as in the *SpekCalc* program, using the Physical Reference Data of NIST (Berger *et al* 2005, Hubbell and Seltzer 1996) for the relevant materials. Spectral predictions were also made using the IPEM78 program, where possible. The IPEM program is limited, however, to a maximum tube potential of 150 kV and a maximum anode angle of 22°. We note that IPEM78 also uses the NIST Reference Data for photon attenuation and absorption.

The predictions of *SpekCalc* are presented in figure 2, along with those of BEAMnrc and, where possible, IPEM78. All the spectra have been assigned 2 keV bin widths and normalized to unit area. The agreement between the three models over a wide range of tube potentials (50–250 kV) and anode angles (10°–24°) generally appears good. The spectral predictions of IPEM78 are, however, consistently slightly harder (more penetrative). This has been observed elsewhere (Poludniowski 2007). Table 1 presents comparisons of HVL_1, HVL_2, E_{mean} and E_{eff}, derived from the spectra. The maximum discrepancy in HVL_1 between BEAMnrc and *SpekCalc* is 3%. The maximum discrepancy in HVL_2 between BEAMnrc and *SpekCalc* is also 3%. In all cases, the HVL predictions of *SpekCalc* are closer to those of BEAMnrc than those of IPEM78. The maximum discrepancies in E_{mean} and E_{eff}, between BEAMnrc and *SpekCalc*, were <2% in both cases. In all cases, except one, the E_{mean} and E_{eff} predictions of *SpekCalc* are closer to those of BEAMnrc than those of IPEM78. In the exception, the difference between the IPEM78 and *SpekCalc* predictions is marginal in any case.

5. Conclusion

A freely available and user-friendly software program was presented for calculating tungsten anode x-ray tube spectra. *SpekCalc* provides predictions almost-instantly, models a wide-range of tube-potentials and provides predictions in satisfactory agreement with state-of-the-art Monte Carlo calculations. The program is of interest to those working with x-ray tubes in diagnostic radiology, radiotherapy and industry, as a research and educational tool.

Acknowledgments

This work was partially supported by research grant C46/A2131 from Cancer Research UK. The project was also partially supported by a teaching innovation grant from McGill University (MTALIF grant). We acknowledge NIHR funding to the NHS Biomedical Research Centre.

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