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Technical Note: SpekPy v2.0—a software toolkit for modeling x-ray tube spectra

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Purpose: SpekPy is a free toolkit for modeling x-ray tube spectra with the Python programming language. In this article, the advances in version 2.0 (v2) of the software are described, including additional target materials and more accurate modeling of the heel effect. Use of the toolkit is also demonstrated.
Methods: The predictions of SpekPy are illustrated in comparison to experimentally determined spectra: three radiation quality reference (RQR) series tungsten spectra and one mammography spectrum with a molybdenum target. The capability of the software to correctly model changes in tube output with tube potential is also assessed, using the example of a GE Revolution™ CT scanner (GE Healthcare, Waukesha, WI, USA) and specifications in the system's Technical Reference Manual. Furthermore, we note that there are several physics models available in SpekPy. These are compared on and off the central axis, to illustrate the differences.
Results: SpekPy agrees closely with the experimental spectra over a wide range of tube potentials, both visually and in terms of first and second half-value layers (HVLs) (within 2% here). The CT scanner spectrum output (normalized to 120 kV tube potential) agreed within 4% over the range of 70 to 140 kV. The default physics model (*casim*) is adequate in most situations. The advanced option (*kqp*) should be used if high accuracy is desired for modeling the anode heel effect, as it fully includes the effects of bremsstrahlung anisotropy.
Conclusions: SpekPy v2 can reliably predict on- and off-axis spectra for tungsten and molybdenum targets. SpekPy's open-source MIT license allows users the freedom to incorporate this powerful toolkit into their own projects. *© 2021 The Authors. Medical Physics published by Wiley Periodicals LLC on behalf of American Association of Physicists in Medicine* [https://doi.org/10.1002/mp.14945]

Key words: software, X-ray imaging, X-ray spectra, X-ray tube modeling

1. INTRODUCTION

Predicting the x-ray spectra emitted from x-ray tubes has a history going back a 100 yr.[1] In the era of the personal computer, this has evolved from an academic pursuit for understanding empirical observation into a practical tool for routine use in hospitals, education, industry, and research. There are a variety of software applications and toolkits available for use in medical physics.[2–7] The choice of tool depends on the precise application and needs of the user, as well as personal inclination. One of the authors of this article was involved in the creation of SpekCalc, a popular application based on a graphical user interface (GUI).[3] SpekPy, the subject of this article, can be seen as a further development providing more powerful functionality and moving beyond the limitations of a graphical interface.

SpekPy is an open-source toolkit for modeling x-ray tube spectra. The code is written in the Python language (Python Software Foundation, DE, USA). SpekPy version 1.0 (v1) was introduced by Bujila et al[8] for modeling x-ray tubes over a wide range of tube potentials (15 to 1000 kV), although it was limited to predictions for tungsten anodes. In this note we summarize the toolkit's core functionality, describe the advances incorporated in SpekPy version 2.0 (v2) and provide examples demonstrating the power of the toolkit. Notably, in v2, molybdenum and rhodium anodes (20–50 kV) can be now be modeled as well as improved tungsten anode spectra (20–300 kV). This means that x-ray tubes relevant to mammography, radiography, low- and medium-energy x-ray radiotherapy, and industrial testing can now all be simulated.

2. MATERIALS AND METHODS

2.A. About the toolkit

The SpekPy toolkit is available free-of-charge under the permissive MIT software license. It is compatible with Python language versions 2 and 3. It requires the standard NumPy and SciPy Python libraries.[9,10] The *matplotlib* library is also useful for plotting results.[11] For installation instructions, see the online software repository (https://bitbucket.org/spekpy/spekpy_release). Currently there is no GUI or web application available and the user is required to input commands. This can be done in a Python script or from a Python interpreter.

SpekPy is written in an object-oriented programming paradigm, using *classes* and *methods*. The name of the main class of the toolkit is Spek. The user creates *instances* of that class and each instance is a representation of a particular x-ray tube. There are several keyword arguments available when creating a spectrum instance. The most important are presented in Table I. A range of additional tools, referred to as class methods, have been provided so that the user of the toolkit can filter x-ray spectra, calculate different x-ray beam metrics, create new materials, save or load SpekPy states, and save or load spectra to or from text files. An overview of the most important class methods is presented in Table II.

An illustration of the use of SpekPy is provided in the appendix. The example script builds a representation of the GE Revolution$^{\text{TM}}$ CT scanner (GE Healthcare, Waukesha, WI, USA), based on information available in the Technical Reference Manual (TRM).[12]

2.B. Physics models in the toolkit

New physics models have been introduced in SpekPy v2, incorporating the advances recently presented by Omar et al.[13–15] Four physics models available in SpekPy v2 are listed in Table III.

TABLE I. The most important keywords that can be specified when an instance of the *Spek* class is created.

Keyword	Comment	Default value
kvp	Tube potential [kV]	100
th	Anode angle, θ [degrees]	12
targ	Target material [“W,” “Mo,” or “Rh”]	“W”
dk	Width of energy bin [keV]	0.5
mas	Exposure setting [mAs]	1.0
physics	Physics model [see Table III]	“casim”
z	Focus-to-detection distance [cm]	100
x / y	Lateral position, anode-cathode/other direction [cm]	0 / 0
obli	Oblique paths in filters considered [True or False]	True
mu_data_source	Source of photon coefficients [“nist” or “pene”]	See Table III

TABLE II. The most important methods for the Spek class.

Method	Category	Description
filter()	G	Apply a filter of specified material and thickness
multi_filter()	G	Apply multiple filters of specified thicknesses
set()	G	Change a keyword parameter for a spectrum instance
clone()	G	Make a copy of a spectrum instance
get_spectrum()	E	Return the fluence spectrum and energy bins
get_kerma()	E	Air kerma
get_hvl1()	E	First half-value layer (material selectable)
get_hvl2()	E	Second half-value layer (material selectable)
get_hc()	E	Homogeneity coefficient (material selectable)
get_emean()	E	Mean energy of the spectrum
get_eeff()	E	Effective energy of the spectrum (material selectable)
get_matl()	E	Thickness for a specified attenuation (material selectable)
get_flu()	E	Integrated fluence of the spectrum
get_eflu()	E	Integrated energy fluence of the spectrum
get_std_results()	E	Standard results such as beam-quality metrics
make_matl()	M	Create new material (by formula or weight fractions)
remove_matl()	M	Delete a material from the database
show_matl()	M	Show the materials available
load_state()	S	Load a previously saved state
save_state()	S	Save a spectrum instance state
remove_state()	S	Permanently remove a state
show_states()	S	Show the available saved states
export_spectrum ()	IO	Export a spectrum to a text file
load_from_file()	IO	Load a spectrum from a text file

Methods are categorized into General (G), Extraction of values (E), Materials (M), States (S), or Input/output (IO). For details of the arguments that can be passed to each method, see the *Function glossary* on the repository’s Wiki pages (https://bitbucket.org/spekpy/spekpy_release/wiki/Function%20glossary).

The *spekcalc* and *spekpy-v1* models were available in SpekPy v1. The *spekcalc* mode (referred to as *legacy* mode in v1) emulates the predictions of the SpekCalc application. The *spekpy-v1* mode was the default model in v1 of SpekPy and incorporated theoretical and numerical improvements to SpekCalc’s approach. The details of the implementations are published elsewhere.[8,16,17] Notably, however, both assume a uniform angular distribution for bremsstrahlung emission and use empirical normalizations to reference data. They also use simple semi-empirical models for the characteristic x-ray contribution (K-shell only for *spekcalc*), without applying any filtering of the characteristic emissions by the target. The default selections for photon coefficients (for both mass attenuation and mass energy absorption) are from the tabulations by the National Institute of Standards and Technology (NIST: MD, USA).[18,19]

The *casim* mode is the new default model in SpekPy v2. The bremsstrahlung contribution is based on simulations of

TABLE III. Physics models available in SpekPy v2.0.

Physics model	Comment	Target types	Photon dataset
casim	Default in SpekPy v2	W, Mo, Rh	PENELOPE
kqp	Highest accuracy model (slower)	W, Mo, Rh	PENELOPE
spekcalc	Emulates the SpekCalc software	W	NIST
spekpy-v1	Previous default in SpekPy v1	W	NIST

Model choice is specified programmatically using the *physics* keyword. The available target material selections are listed for each model. The default selections for photon coefficients (for both mass attenuation and mass energy absorption) are also stated, where NIST refers to National Institute of Standards and Technology (MD, USA) and PENELOPE refers to the PENELOPE Monte Carlo code system.[21]

electron direction, as well as energy, at depth in the target. Tabulated grids for incident electron in the range 20–300 keV are taken from the work of Omar et al.[14] The NIST tabulations of the bremsstrahlung cross-sections differential in photon energy[20] are used (as in *spekpy-v1* but not *spekcalc*). A simple approximation for the bremsstrahlung angular distribution is applied. The *casim* model is identical to the *sim* model described in Omar et al.,[14] for spectra on the central axis. For off-axis spectra, however, although variable self-filtration of the anode is accounted for, the integration over the bremsstrahlung angular distribution is not recalculated at different emission angles. This allows rapid calculation of metrics at multiple spatial points for the same tube instance, for example, when calculating an air kerma profile. The characteristic contribution is based on the Monte Carlo calculated depth distributions in the target anode presented by Omar et al.[13] Both L and K shells are included and the appropriate emission angle-dependent target filtration is applied. The default selections for photon coefficients (for both mass attenuation and mass energy absorption) are derived from the PENELOPE Monte Carlo code system.[21]

The *kqp* mode, also introduced in SpekPy v2, is the most accurate model, representing a full implementation of the innovations suggested in Omar et al.[14,15] There are two differences to the default *casim* mode. First, it uses a parameterization of the bremsstrahlung angular distribution due to Kissel, Quarles, and Pratt,[22] rather than relying on a simplified expression. Second, the *kqp* mode recalculates the integration over the bremsstrahlung angular distribution for each emission angle as well as applying angle-dependent target self-filtration.

Both the *casim* and *kqp* models now also offer the possibility of simulating molybdenum and rhodium targets, in addition to tungsten. For the bremsstrahlung contributions, the electron depth-distribution data published in Omar et al.,[23] are used for molybdenum and tungsten. Rhodium electron depth-distributions are estimated by scaling those of molybdenum by the ratios of the materials' continuous slowing down approximation (CSDA) ranges. This is a reasonable approximation due to the similar atomic number of the two materials. For the characteristic contributions, the simulated depth-distribution data published in Omar et al.,[24] are used for all three target materials.

2.C. Toolkit demonstration

2.C.1. Predicting the output and half-value layer of a tube

The HVL and CT dose index free in air[25] ($\mathrm{CTDI}_{\text{free air}}$) were predicted for a GE Revolution™ CT scanner at several x-ray tube potentials. The representation of the CT scanner was constructed by matching the nominal HVL at a tube potential of 120 kV. We further exploit the fact that $\mathrm{CTDI}_{\text{free air}}$ is proportional to air kerma at the isocenter and that the conversion factor between them can be treated as independent of tube voltage for a fixed beam collimation. The air kerma predictions of SpekPy were multiplied by a conversion factor determined based on the nominal specification of $\mathrm{CTDI}_{\text{free air}}$ for 120 kV and 40 mm collimation. The HVL and $\mathrm{CTDI}_{\text{free air}}$ predictions of SpekPy at tube voltages of 70, 80, 100, and 140 kV were then compared with the nominal specifications in the TRM. See the Appendix for details of the implementation.

2.C.2. Comparison to experimental spectra

Predictions of SpekPy were compared to a variety of published spectra, in terms of the fluence spectra and HVLs (in mm of aluminium).

Radiography spectra were selected from data published by a national standard laboratory.[26] The x-ray tube had a tungsten anode and a 20 degree anode angle. The tube had inherent filtration of 1 mm beryllium (window) and 250 μm Kapton (monitor chamber). Additional filtration was 2.5 mm of aluminium. Measurements presented are for three spectra corresponding to three tube potentials: 60 kV (RQR4), 80 kV (RQR6), and 120 kV (RQR9). The measurements were performed on the central axis at a focus-to-detector distance of 100 cm.

A single mammography spectrum was selected, generated using a Hologic Selenia DR mamography system with a molybdenum anode.[27] The spectrum was filtered with 0.8 mm beryllium and 25 μm of rhodium. The anode angle was 22.4 degrees and the tube potential was 28 kV. The presence of a 45 cm air gap and a compression paddle of 2.35 mm PMMA was also assumed. There is a spuriously high low-energy tail in the measured spectra.[15] To suppress this, 10 mm of adipose tissue[28] was added to both measured and predicted spectra.

The HVLs for the four measured spectra were calculated using SpekPy, after importing the spectra from text files.

2.C.3. Comparison of physics models

For the RQR6 spectrum, the predictions of the four SpekPy physics models listed in Table III were compared. Air kerma predictions on and off the central axis were also calculated for all three RQR spectra.

3. RESULTS

3.A. Predicting the output and half-value layer of a tube

The HVL and $CTDI_{free\ air}$ predictions for the SpekPy representation of a GE Revolution^{TM} CT scanner are presented in Table IV. The HVLs agree within the stated precision of the TRM and the $CTDI_{free\ air}$ predictions are within 4%.

TABLE IV. Calculated 1st HVL and $CTDI_{free\ air}$ values for five x-ray tube potentials, using the SpekPy model of a GE Revolution^{TM} CT scanner.

Tube potential (kV)	HVL1 (SpekPy) (mm Al)	HVL1 (Ref.) (mm Al)
70	4.7	4.7
80	5.4	5.4
100	6.6	6.6
120	7.6	7.6
140	8.5	8.5

Tube potential (kV)	$CTDI_{free\ air}$ (SpekPy) (mGy/400 mAs)	$CTDI_{free\ air}$ (Ref.) (mGy/400 mAs)
70	18.08	18.76
80	26.74	27.47
100	48.67	49.19
120	75.81	75.81
140	107.22	106.88

Reference values are taken from the Technical Reference Manual for the "Large" collimator filter and 40 mm collimation.[12] HVL and $CTDI_{free\ air}$ predictions were matched to the reference values at a tube potential of 120 kV. The SpekPy physics model was the default selection (*casim*)

3.B. Comparison to experimental spectra

The four experimental mammography and radiography spectra and SpekPy predictions are presented in Fig. 1. The SpekPy predictions have been convolved with a Gaussian filter to provide similar energy resolution to the detector measurements. Visually, the agreement of SpekPy with experiment is good. The calculated first and second HVLs are provided in Table V. The agreement is excellent, matching to within 2% in all cases.

3.C. Comparison of physics models

The results presented previously were generated using SpekPy's default *casim* physics model. The differences between the available physics choices are highlighted in Fig. 2. In the figure, the predictions of the RQR6 spectrum are plotted for all the four models listed in Table III. The *casim* model predictions are closely coincident with those of the most accurate model: *kqp*. The *spekcalc* model, however, over predicts the fluence at the high-energy tail. The overprediction is worse still for the *spekpy-v1* model.

Air kerma predictions along the anode–cathode are presented in Fig. 3 for the three RQR spectra, at a 100 cm focus-to-detection distance. The values for each spectrum are normalized by the associated central-axis fluence (i.e., fluence at $x = 0$). The values calculated from the experimental spectra on the central axis are also displayed. The predictions off-axis include the effects of distance squared, the oblique path of x-rays through any filters and the anode heel effect. The

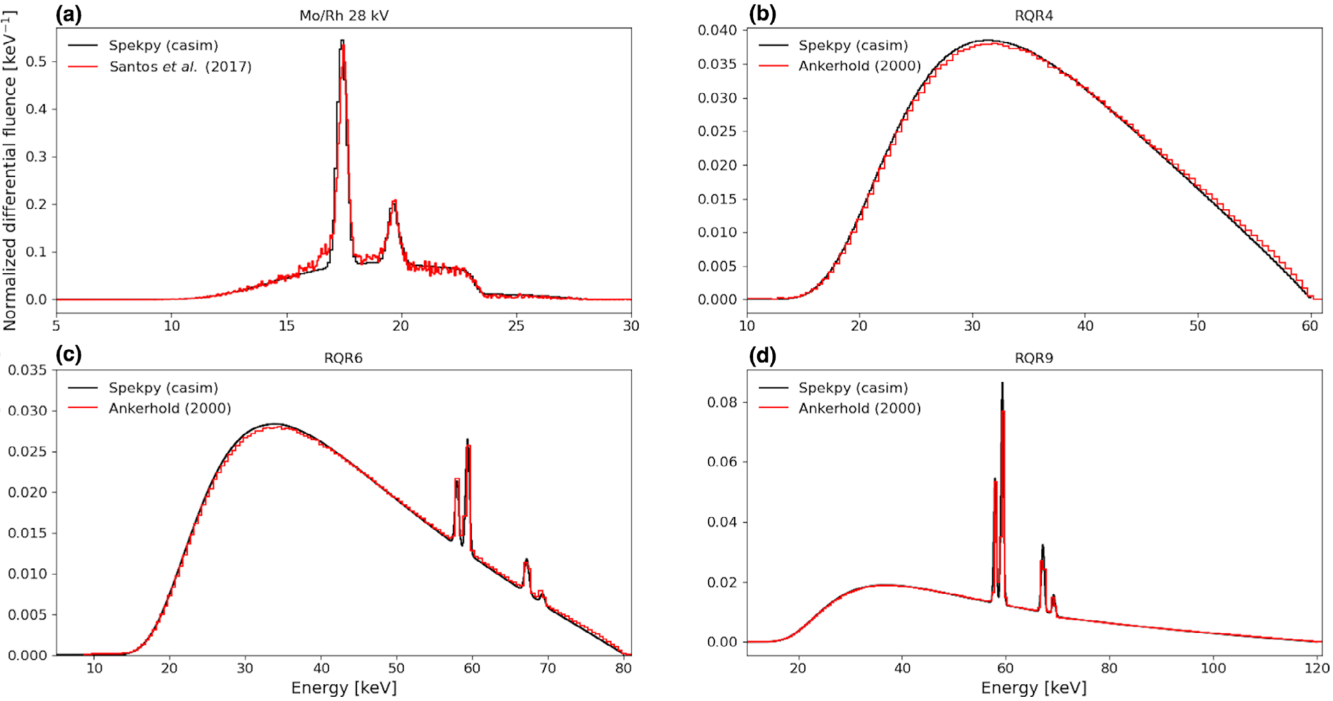

FIG. 1. Comparisons of SpekPy predictions (*casim*) with experimental determinations: (a) Mo/Rh 28 kV (Santos et al.[27]), (b) RQR4 (Ankerhold[26]), (c) RQR6 (Ankerhold), and (d) RQR9 (Ankerhold). The areas under the curves are normalized to unity. The bin width for the SpekPy calculations was 0.1 keV with a Gaussian filter of $\sigma = 0.2$ and 0.25 keV applied, for mammography and radiography spectra, respectively. The Gaussian filter was applied using functionality inbuilt to SpekPy. [Color figure can be viewed at wileyonlinelibrary.com]

TABLE V. Calculated first and second HVL values for four spectra (Mo/Rh 28 kV, RQR4, RQR6, and RQR9) using the *casim* physics model

Spectrum	HVL1 (SpekPy) (mm Al)	HVL1 (Ref.) (mm Al)	Discrepancy (%)
Mo/Rh 28	0.498	0.491	1.4
RQR4	2.042	2.051	−0.5
RQR6	2.631	2.637	−0.2
RQR9	3.955	3.938	0.4

Spectrum	HVL2 (SpekPy) (mm Al)	HVL2 (Ref.) (mm Al)	Discrepancy (%)
Mo/Rh 28	0.570	0.560	1.8
RQR4	2.840	2.888	−1.7
RQR6	3.951	4.012	−1.5
RQR9	6.393	6.433	−0.6

Reference values were calculated based on experimentally determined spectra (Ankerhold[26] and Santos et al.[27])

kqp predictions can be considered the benchmark. Two observations that can be made are that *spekcalc* curves are displaced upwards from the rest and that the *kqp* curves exhibit a different shape to the others.

4. DISCUSSION

The example predictions for the GE Revolution CT scanner indicate that using a one-time matching at a single tube potential, good agreement for HVL and $CTDI_{free\ air}$ at different tube potentials can be expected (see Table IV). This supports the conclusions of Omar et al.,[15] that the models underlying SpekPy v2 accurately describe the change in fluence as well as the change in spectral shape with tube potential.

For the four spectra plotted in Fig. 1 and the derived HVLs presented in Table V, there was good agreement between SpekPy and experiment, with the HVLs matching within 2%. Note that the new SpekPy v2 models utilize the photon cross-sections derived from the PENELOPE Monte Carlo code system[21] to filter spectra and calculate HVL. These cross-sections were also used for calculation of the HVLs from the experimental spectra. HVL values calculated using the NIST dataset instead varied by up to 2% from those quoted, but provided a similar agreement between experiment and SpekPy, when consistently selected for both.

At the photon energies of kV x-rays, PENELOPE and NIST datasets differ practically only in the data for the photoelectric effect, these being renormalized subshell cross-sections in PENELOPE[29] and unrenormalized cross-sections in NIST based on the XCOM code[18] and the work on mass energy-transfer and mass energy-absorption coefficients by Seltzer.[19] ICRU Report 90 examines both datasets but, unlike for other key data in the report, no specific recommendation is given for one dataset or the other.[30] SpekPy therefore allows the selection of either by the user.

The differences between the available physics choices shown in Fig. 2 can be explained by reference to the underlying physics models. The *spekcalc* option over predicts the fluence at the high-energy tail as does the *spekpy-v1* model. The origin of the over-estimation in both cases is the assumption of *instant electron diffusion* in the anode.[14] In the case of *spekcalc*, however, the error is partially canceled by systematic errors in the bremsstrahlung cross-section (the modified Elwert-Bethe-Heitler cross-section used in SpekCalc is softer than the more accurate NIST cross-section[17]). It can be said, therefore, that *spekcalc* has generally benefited from a

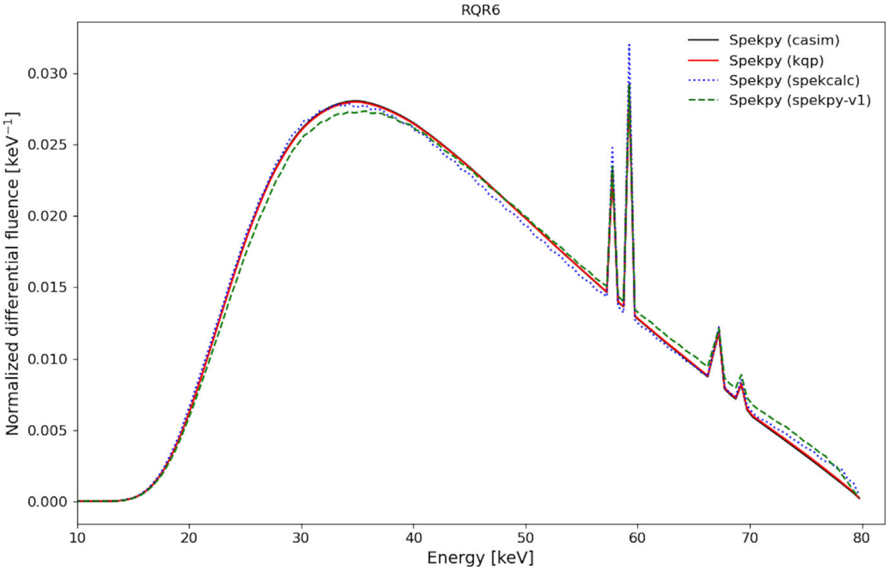

FIG. 2. Predictions of the RQR6 spectrum for various SpekPy models: *casim*, *kqp*, *spekcalc*, and *spekpy-v1*. The area under the curves are normalized to unity. The bin width for the SpekPy calculations is 0.5 keV. [Color figure can be viewed at wileyonlinelibrary.com]

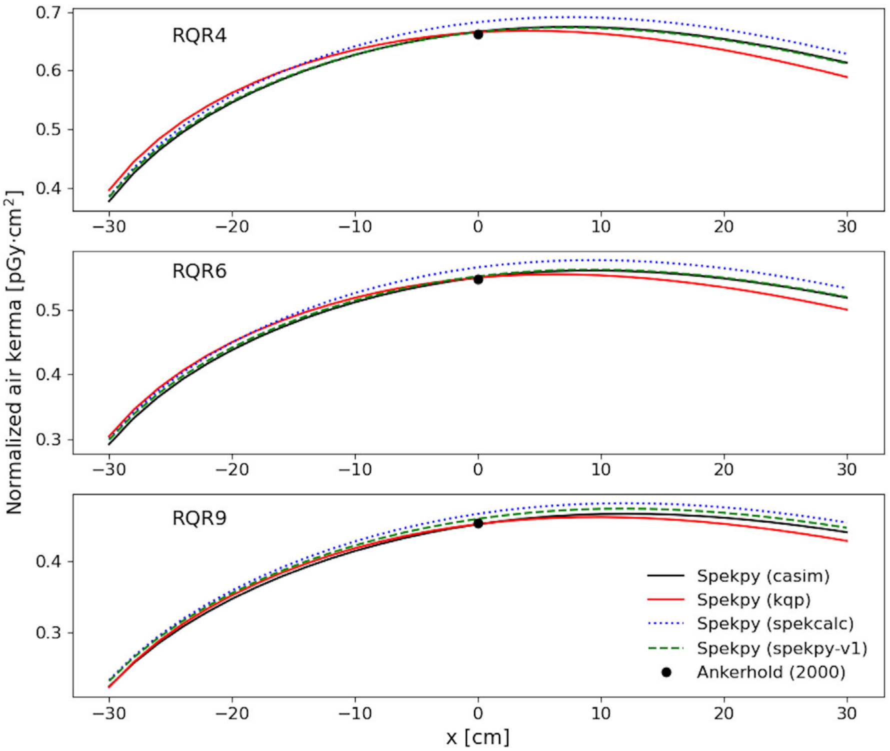

FIG. 3. Normalized air kerma predictions varying with position (anode–cathode direction) for various SpekPy models for RQR4, RQR6, and RQR9 spectra. The models are: *casim*, *kqp*, *spekcalc,* and *spekpy-v1.* Air kerma values are normalized in each case by the total fluence on the central axis ($x = 0$ cm). Values derived from central-axis experimental spectra (using the PENELOPE photon coefficients) are also shown. [Color figure can be viewed at wileyonlinelibrary.com]

fortuitous cancelation in errors. We note that the overestimations in the high-energy tail do not greatly affect HVL predictions and that in this respect *spekpy-v1* was well-validated against measurements.[8]

Two observations were made regarding the air kerma predictions presented in Fig. 3: the *spekcalc* curves are displaced upwards from the rest and the *kqp* curves display a different shape. The first effect (upwards displacement) is primarily due to the use of the NIST coefficients in the *spekcalc* model rather than those derived from the PENELOPE code system. The discrepancy is consistent with the reported difference in the mass energy-absorption coefficient for air when using renormalized (PENELOPE) compared to unrenormalized (NIST) photoeffect cross-sections (see figure 7.4 in ICRU Report 90[30] where the renormalized coefficient is up to 3% lower).

The second effect (curve shape) is due to the fact that *kqp* is the only model to re-evaluate an integral over electron direction and bremsstrahlung angular distribution in the target at each angle of emission. This is more accurate than the approach in the default *casim* model, but is less computationally efficient for calculation of off-axis metrics. On the desktop computer used for the present calculations (Intel i7-4790 3.6 GHz processor), for one spatial position of the RQR6 spectrum, the *casim* model took 0.4 s to generate a spectrum and return an air kerma value, compared to 1.6 s for *kqp*. However, for the 31 positions used to generate the kerma profile, the *casim* model required a total of only 0.5 s, compared to 52.1 s for *kqp*. For a densely sampled line profile or the simulation of a two-dimensional image, the *casim* model therefore provides a dramatic speedup, at the expense of an inaccuracy of up to several percent in modeling the heel effect.

SpekPy v2 contains the most advanced models that we are aware of in any spectrum simulation software for medical x-ray tubes, excepting those resorting to Monte Carlo methods. However, as demonstrated in Omar et al.,[15] other simpler software are perfectly adequate for prediction in many situations. Such a situation is when beam metrics are only required on the central axis for tubes with anode angles typical for most radiology applications (10 to 15 degrees for tungsten anodes). The preferred choice of software will then depend on the user's task and personal preference. A portable application with a simple user interface might be sufficient.[2–4] Alternatively, a scriptable toolkit, such as SpekPy, might be desired.

An alternative toolkit for x-ray spectra calculations available in the Python programming language, with an in-built GUI available, is *xpecgen*.[6] In addition, there are some toolkits available within the MATLAB programming environment (MathWorks Inc., Natwick, WY, USA), such as Spektr[5] and xrTk,[7] with the former also including GUI functionality. All of these toolkits have strengths, although none is as well-suited as SpekPy for the calculation of off-axis spectra.

As a general-purpose toolkit for modeling medical x-ray tubes, the accuracy of SpekPy is probably close to the limit achievable, given the uncertainties in the photon mass attenuation and energy-absorption coefficients and the presence of scatter and off-focal radiation. It should be noted that SpekPy (and other deterministic spectrum software) only provide predictions of primary radiation. If off-focal radiation or scatter must be modeled, Monte Carlo simulation is a preferred approach.

5. CONCLUSION

SpekPy v2 is a powerful free toolkit for modeling x-ray spectra in the Python programming environment. It is based on models that can reliably predict off-axis spectra as well as those on the central axis for tungsten and molybdenum targets. SpekPy's permissive open-source license allows the user great freedom in incorporating the toolkit into their own projects.

ACKNOWLEDGMENTS

We thank Prof. Paulo Costa for providing the x-ray spectra data by Santos et al.[27]

CONFLICT OF INTEREST

The authors have no conflicts to disclose.

APPENDIX A

BUILDING A SPECTRUM MODEL FOR A CT SCANNER

The following script is divided into nine short code sections. It builds a representation corresponding to the GE Revolution^{TM} CT scanner for the "Large" collimator filter, 40 mm collimation, and a 120 kV tube potential. The HVLs and $CTDI_{free\ air}$ are then predicted for other tube potentials and printed to screen.

The initial spectrum instance (section #2) is based on an anode angle of 10.5 degrees and a source-to-detection distance of 62.56 cm, as specified in the scanner's Technical Reference Manual (TRM).[12] Note that an adjustment is found to match the nominal HVL at a tube potential of 120 kV (section #5). This adjustment was 2.41 mm Al and presumed to be necessary to compensate for filtration missing in the TRM specification.

A conversion factor is calculated to normalize from predicted air kerma to nominal $CTDI_{free\ air}$. This factor (calculated as 1.21 in section #8) compensates for any difference from the predicted tube output, as well as the departure of the in-air dose profile of the scanner from the nominal 40 mm width (see the definition of CTDI).[25]

```
# 1. Import the SpekPy toolkit
import spekpy as sp

# 2. Generate a spectrum based on TRM specifications
s = sp.Spek(kvp=120, th=10.5, z=62.56)

# 3. Define and apply the tube filtration specified in TRM
tube_filtration = 3.9
s.filter('Al',tube_filtration)

# 4. Define and apply the "Large" collimator filter specified in TRM
collimator_filtration = [('C',1.94), ('Al',0.19), ('Cu',0.07)]
s.multi_filter(collimator_filtration)

# 5. Make an adjustment (in mm Al) to match the HVL stated in TRM
extra_filtration = s.get_matl(matl='Al',hvl=7.6)
s.filter('Al',extra_filtration)

# 6. Define the reference CTDI(free,air) from the TRM (mGy/400 mAs)
CTDI_ref = 75.81

# 7. Calculate the air kerma (uGy) and convert to mGy/400 mAs
k120 = s.get_kerma(mas=400) * 1e-3

# 8. Calculate air kerma to CTDI conversion factor
conversion_factor = CTDI_ref / k120

# 9. Loop through tube potentials; calculate and print predictions
for pot in [70, 80, 100, 120 ,140]:
    s.set(kvp=pot)
    CTDI = conversion_factor * s.get_kerma(mas=400) * 1e-3
    hvl = s.get_hvl1()
    print(pot, "kV", hvl, "mm Al", CTDI, "mGy/400 mAs")
```

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in SpekPy at https://bitbucket.org/spekpy/spekpy_release, reference number b5e01a8 (v2.04).

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