X-ray machine spectrometry for dosimetry: spectrum modelling

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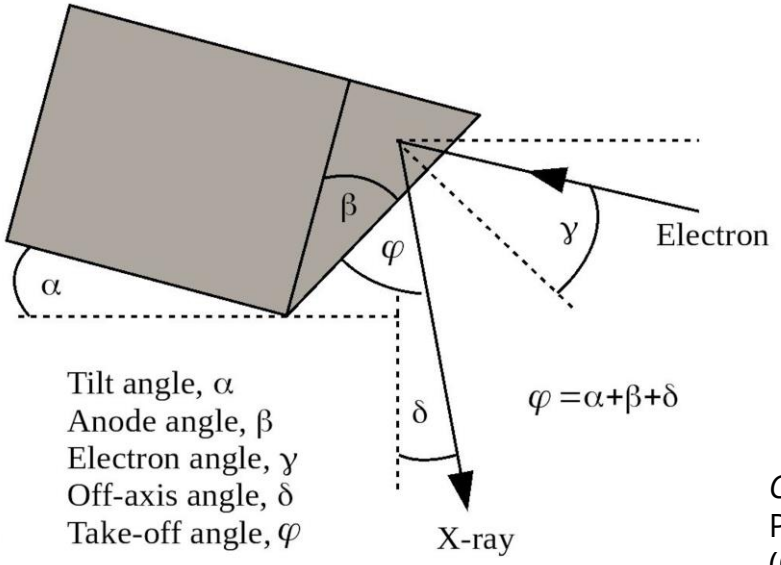
Types of spectrum model

- Monte Carlo simulation
  - Purpose-written e.g. Seltzer and Berger (1970)
  - General purpose e.g. EGSnrc/BEAMnrc, PENELOPE etc.
- Analytical models
  - Empirical e.g. Boone and Seibert (1997), Hernandez and Boone (2014)
  - Semiempirical e.g. Kramers (1923), Birch and Marshall (1979) etc.
  - Theory/simulation hybrid e.g. Omar et al (2020a, 2020b)

The most common type of models for "quick and easy" calculations

Starting point for models: consider a lump of metal



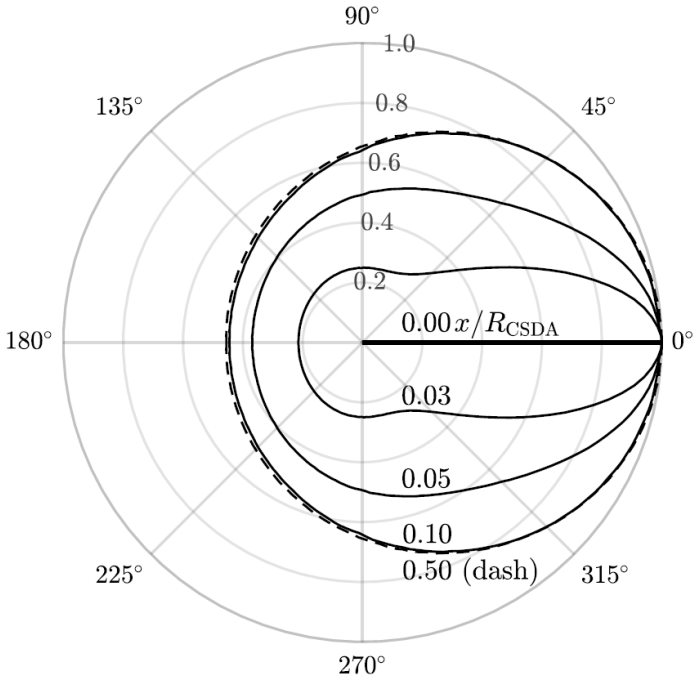
Calculating X-ray Tube Spectra, Chapter 2
Poludniowski, Omar and Andreo
(CRC Press, 2022)

- Models typically assume no tube tilt (α = 0) and provide predictions on the central axis of the beam (δ = 0) for a specified anode angle (β)
- In fact, however, the ”takeoff” angle, φ, is the critical parameter in most models (it determines the self-filtration by the anode)
- If you determine the takeoff angle for your setup, you can input it as an effective anode angle into the model: $\beta_{eff} = \varphi = \alpha + \beta + \delta$

The physics behind x-ray tube models

Electrons hit the anode with energy proportional to the tube potential

- The electrons repeatedly scatter elastically, changing their direction



Calculating X-ray Tube Spectra, Chapter 3
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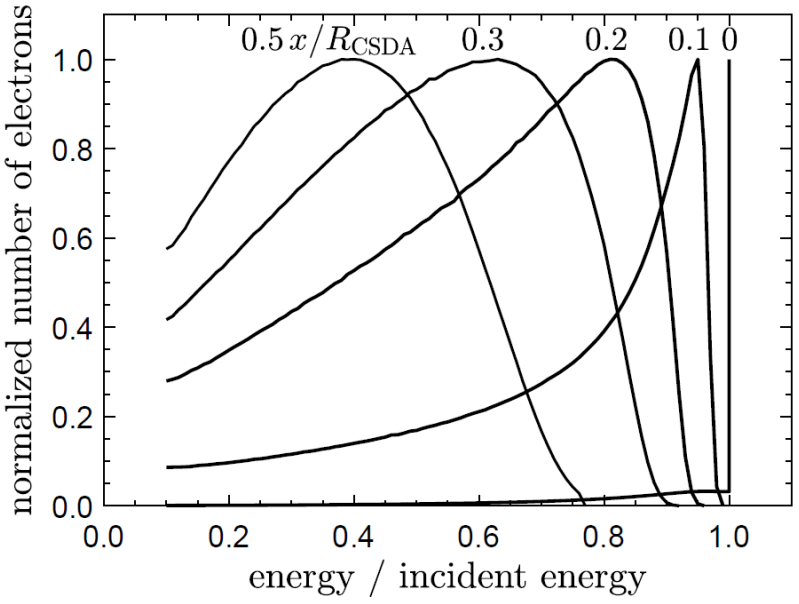
The physics behind x-ray tube models

Electrons hit the anode with energy proportional to the tube potential

- The electrons also lose energy though inelastic collisions



Calculating X-ray Tube Spectra, Chapter 3
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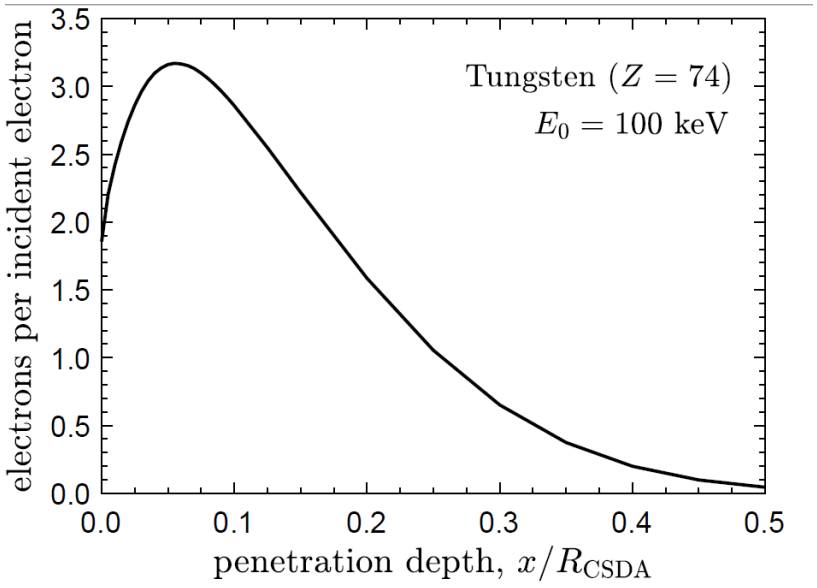
The physics behind x-ray tube models

Electrons hit the anode with energy proportional to the tube potential

- The electrons may penetrate up to about half their CSDA range
- Many electrons backscatter out of the target (~50% in tungsten)



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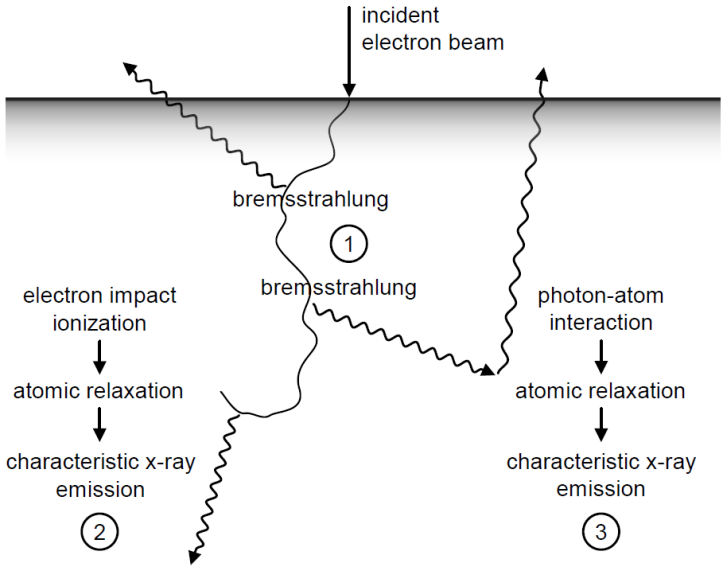
The physics behind x-ray tube models

Electrons hit the anode with energy proportional to the tube potential

- The electrons emit bremsstrahlung radiation (~1% of their energy, but dependent on tube potential and target atomic number)



Calculating X-ray Tube Spectra, Chapter 3
Poludniowski, Omar and Andreo
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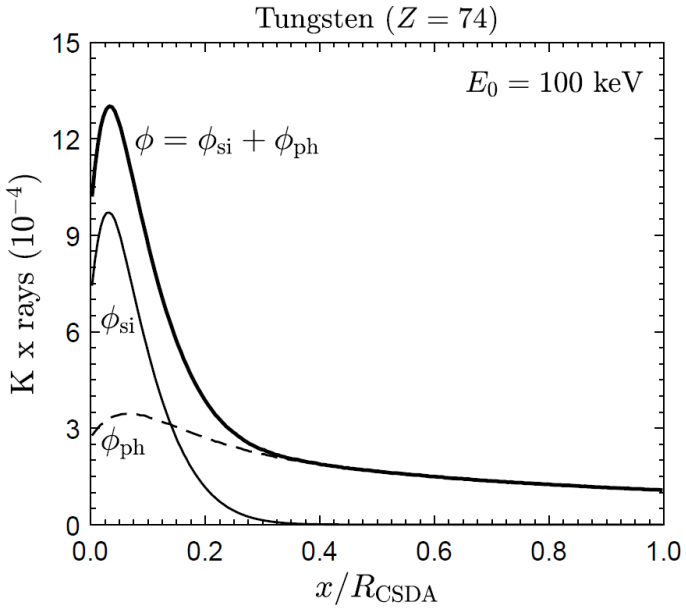
The physics behind x-ray tube models

Electrons hit the anode with energy proportional to the tube potential

- If sufficiently energetic, the electrons produce characteristic emissions in the target via electron impact ionization
- If the bremsstrahlung is sufficiently energetic, self-filtration (reabsorption) will also result in further characteristic emissions



Φ_{si} – impact ionization contribution
Φ_{ph} – photon-atom contribution

Calculating X-ray Tube Spectra, Chapter 3
Poludniowski, Omar and Andreo
(CRC Press, 2022)

Limitations of the analytical models

Approximation	1st order	2nd order	3rd order
Electrons penetrate in straight lines (literally or effectively)	Yes	Yes	No
Electrons lose energy deterministically as they penetrate the target	Yes	No	No
Fitted/empirical bremsstrahlung cross-section	Yes (mostly)	No	No
Uniform bremsstrahlung angular distribution	Yes	Yes	No

- **1st order models**: Kramers (1923), Soole (1976), Birch and Marshall (1979), Tucker-Barnes (1991), IPEM Report 78 (1995), Blough et al (1998)
- **2nd order models**: SpekCalc (2009), Hernandez and Fernandez (2016) and SpekPy V1(2020)
- **3rd order models**: SpekPy V2 (2021)

What is SpekPy?

- SpekPy is a free software toolkit for calculating and manipulating x-ray tube spectra.
- It probably has the most advanced physics models in any spectrum software, excepting full Monte Carlo treatment
- The code is written in the Python programming language
- SpekPy is a toolkit rather than an application so you will need to write/run simple Python scripts
- Fortunately, there is an extensive list of short example scripts in the online repository to get you started

Git repository and Wiki: https://bitbucket.org/spekpy/spekpy_release

Using SpekPy

Installation (all free):

- Python 3
- NumPy, SciPy and optionally *matplotlib* (all standard libraries)
- SpekPy (from https://bitbucket.org/spekpy/spekpy_release)

Information you will need:

- Tube potential [kV]
- Anode angle [degrees]
- Filtration [mm of materials]
- Position to evaluate spectrum [x-y-z, cm]

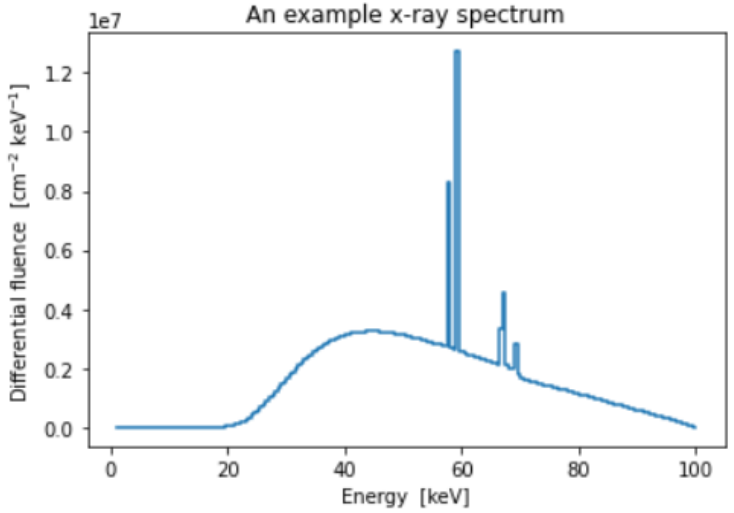
Note:

- Not everyone thinks about the anode/tilt angles when they specify beams, but it is important for accurate modelling
- Remember: filtration by air can be important for low kV beams

Example

```python
import spekpy as sp # Import the SpekPy library for spectral calculations
import matplotlib.pyplot as plt # Import pyplot for plotting

print('\nRunning demo script (1 mAs, 100 cm)\n')

## Generate spectrum for 100 kV potential, 10 deg. anode angle & 6 mm Al filtr.
s=sp.Spek(kvp=100.,th=10.) # Create the spectrum model
s.filter('Al',6.) # Add the filtration [mm]
k, phi_k = s.get_spectrum(edges=True) # Get arrays of energy & fluence spectrum

## Calculate metrics (1 mAs, 100 cm source-to-detector distance)
hvl1 = s.get_hvl1() # Get 1st HVL
hvl2 = s.get_hvl2() # Get 2nd HVL
kair = s.get_kerma() # Get air kerma
phi = s.get_flu() # Get total fluence

## Print metrics to screen
print('HVL1:',round(hvl1,2),'mm Al')
print('HVL2:',round(hvl2,2),'mm Al')
print('Kair:',round(kair,2),'uGy')
print('Fluence:',"{:e}".format(phi),'cm-2')

## Plot the x-ray spectrum
plt.plot(k, phi_k)
plt.xlabel('Energy  [keV]')
plt.ylabel('Differential fluence  [cm$^{-2}$ keV$^{-1}$]')
plt.title('An example x-ray spectrum')
plt.show()

print('\nFinished!\n')
```

```
Running demo script (1 mAs, 100 cm)

HVL1: 5.5 mm Al
HVL2: 7.19 mm Al
Kair: 57.48 uGy
Fluence: 1.502284e+08 cm-2
```




```
Finished!
```

Some of the functions available

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

SpekPy physics models

Default →

Best →

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

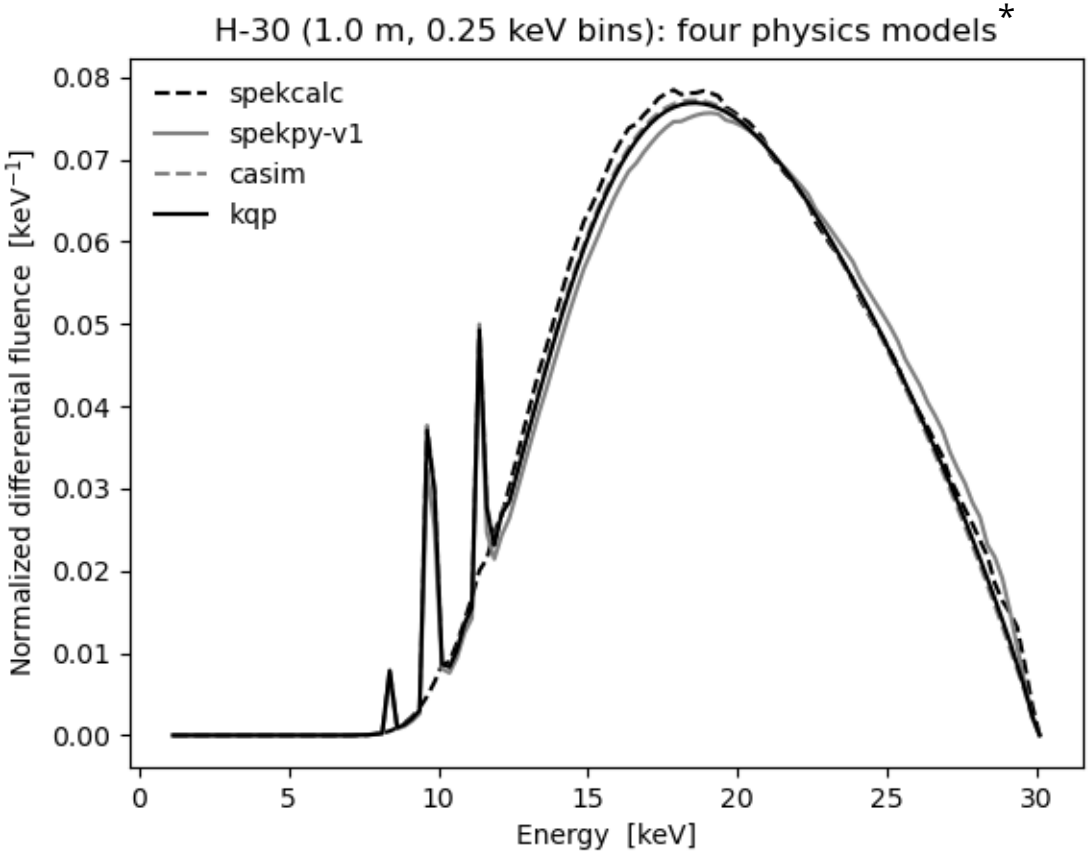
Physics model	Comment	Target types	Photon dataset
casim	Default in SpekPy v2	W, Mo, Rh	PENELOPE
kqp	Highest accuracy model (slower)	W, Mo, Rh	PENELOPE
spekcalc	Emulates the SpekCalc software	W	NIST
spekpy-v1	Previous default in SpekPy v1	W	NIST

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]

SpekCalc *vs* SpekPy V1 *vs* SpekPy V2

- SpekCalc slightly overestimates the spectrum in the high-energy tip
- SpekCalc does not model L-lines and therefore is inaccurate for lightly filtered spectra at low tube potentials, e.g. H-30 etc.
- SpekPy V1 includes L-lines and generally provides good HVL predictions, but the overestimation in the high-energy tip is worse than SpekCalc
- Neither SpekCalc nor SpekPy V1 accurately model the anode heel effect
- Neither SpekCalc nor SpekPy V1 accurately model the self-filtration of characteristic x-rays
- SpekPy V2 can model HVLs, fluence and heel effect accurately for both bremsstrahlung and characteristic x-rays (compared to Monte Carlo)
- Use the “kqp” model of SpekPy V2 if you want the very highest accuracy (this is recommended for modelling the heel effect)

SpekCalc *vs* SpekPy V1 *vs* SpekPy V2



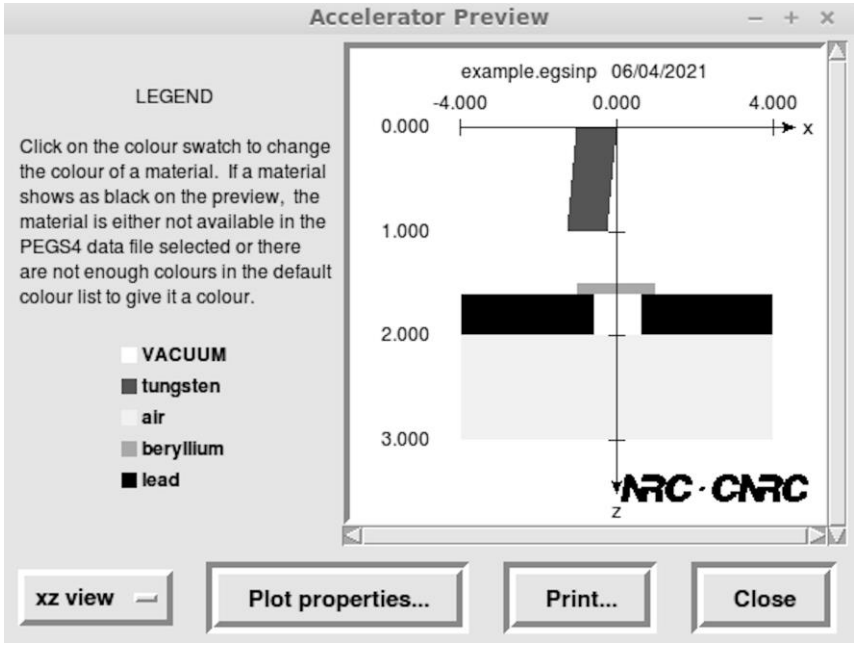

```
HVL1(spekcalc): 0.413 mm Al
HVL1(spekpy-v1): 0.385 mm Al
HVL1(casim): 0.371 mm Al
HVL1(kqp): 0.373 mm Al

HVL1(ISO 4037-1): 0.364 mm Al
```

*20 degree anode angle is assumed

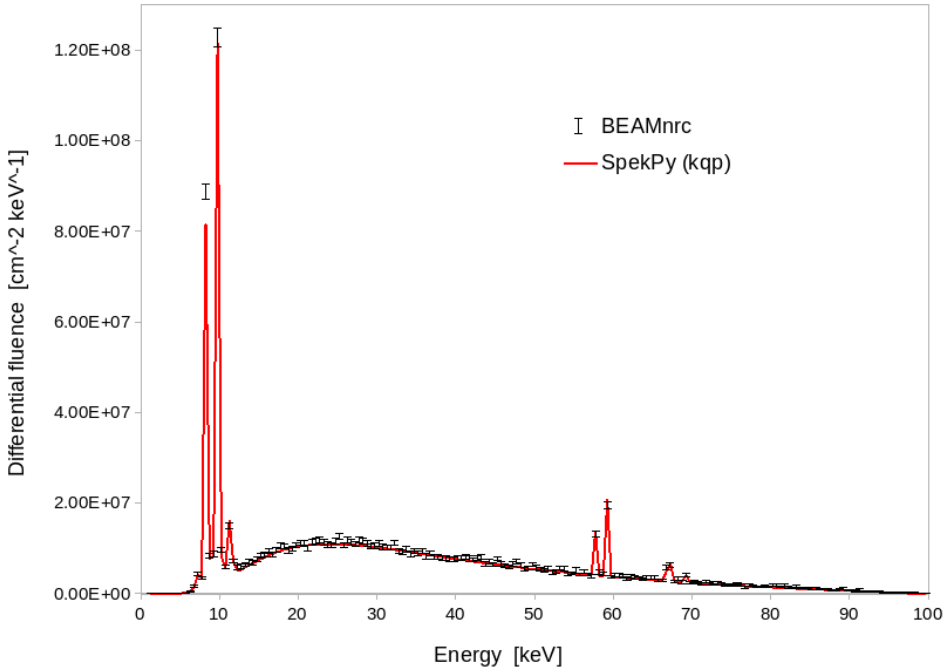
Comparison to Monte Carlo

Scenario: 100 kV, 14º anode angle, 1 mm Be, air column, 100 cm SDD

EGSnrc/BEAMnrc



Comparison with SpekPy V2 (kqp)



Chapter 7: https://bitbucket.org/caxtus

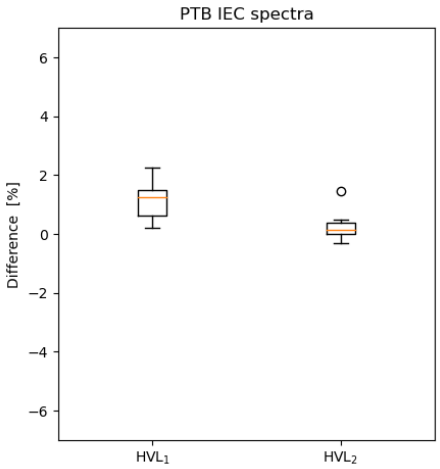
Half-value layer comparison

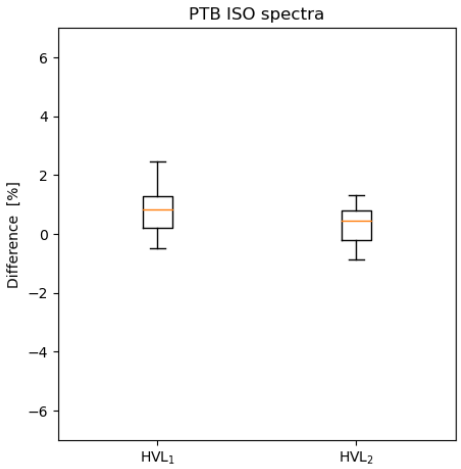
PTB: 18 IEC spectra [RQR2-10, RQA2-10] (Ankerhold 2000, spectrometry)

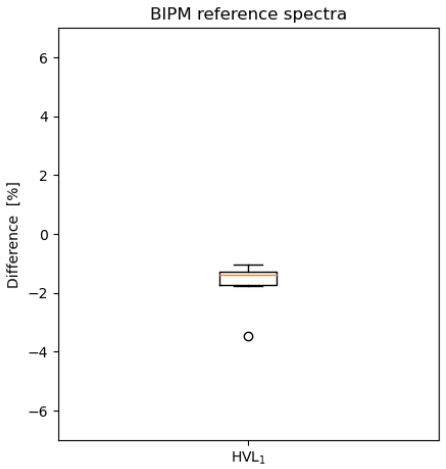
PTB: 29 ISO spectra [Hx6, Wx7, Nx9, Lx7] (Ankerhold 2000, spectrometry)

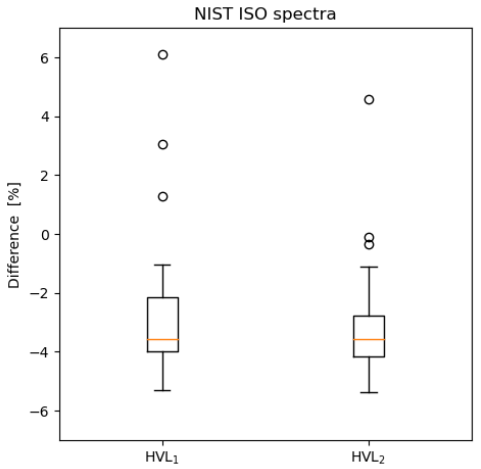
BIPM: 15 reference spectra [tungsten] (Kessler and Burns 2018, dosimetry)

NIST: 29 ISO spectra [HKx6, WKx7, NKx9, LKx7] (O'Brien 2017, dosimetry)









Mean +/- std	HVL1: 1.2 +/- 0.5% HVL2: 0.2 +/- 0.4%	HVL1: 0.8 +/- 0.8% HVL2: 0.4 +/- 0.6%	HVL1: -1.6 +/- 0.6%	HVL1: -2.7 +/- 2.4% HVL2: -3.0 +/- 2.0%

Chapter 8: https://bitbucket.org/caxtus

Half-value layer accuracy

- Is this good enough?
- That’s for you to decide (it depends on the task)
- To put the numbers is context: it has been suggested that best estimate of filter thickness that can be achieved with reasonable effort is limited to 3% or 10 µm (whichever is greatest)*

*ISO 4037-1:2019, Section 4.2.4

Half-value layer matching

- Residual discrepancies can be eliminated by using the function **`get_matl()`**.
- This can be used to find the material thickness that you need to add (or subtract) to match the HVL1 exactly
- Of course, the HVL2 will still likely not match exactly, but it should also be very close

Current limitations

- Narrow-beam only
  - This won't change!
- Targets: W, Mo, Rh
  - We may add other targets (e.g., Cu)
- The target material is considered pure
  - No plans to consider tungsten-rhenium alloys, but we could do so
- Tube potentials: 20-300 kV (W), 20-50 kV (Mo, Rh)
  - Planned extension (down to 10 kV and up to 500 kV for W)
- A constant tube potential is assumed with zero ripple
  - No plans to include ripple, but we could do so
- Currently there is no graphical interface
  - But a web app will be made available very soon!

For more information on SpekPy V2: technical papers on the model

- Omar A, Andreo P, Poludniowski G. *Performance of different theories for the angular distribution of bremsstrahlung produced by keV electrons incident upon a target*. Radiat. Phys. Chem. 2018;148:73-85
- Omar A, Andreo P, Poludniowski G. *A model for the emission of K and L x rays from an x-ray tube*. Nucl Instrum Methods Phys Res B. 2018;437:36-47
- Omar A, Andreo P, Poludniowski G. *A model for the energy and angular distribution of x rays emitted from an x-ray tube*. *Part I. Bremsstrahlung production*. Med Phys. 2020;47(10):4763-4774
- Omar A, Andreo P, Poludniowski G. *A model for the energy and angular distribution of x rays emitted from an x-ray tube*. *Part II. Validation of x-ray spectra from 20 to 300 kV*. Med Phys. 2020;47(9):4005-4019

For more information on SpekPy V2: toolkit, background and examples

https://doi.org/10.1002/mp.14945

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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.

[https://doi.org/10.1002/mp.14945]

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

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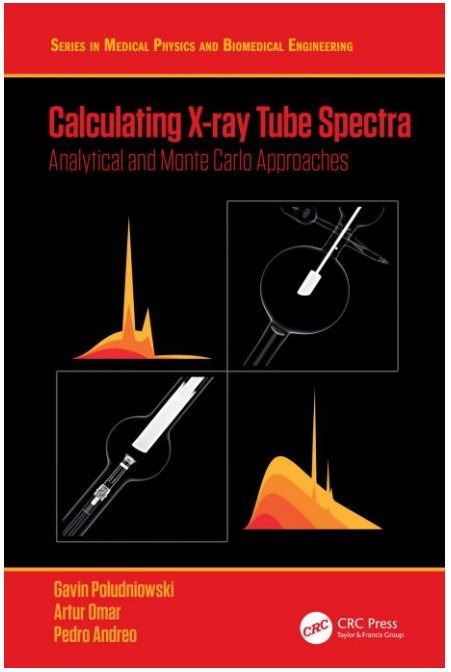

You can access accompanying code examples for free here: https://bitbucket.org/caxtus

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