An introduction to USpekPy package

Uncertainty estimation on protection quantities for x-rays using SpekPy and Monte Carlo techniques

Xandra Campo

Ionizing Radiation Metrology Laboratory (LMRI)
CIEMAT, Spain

June 2024

Table of Contents

- Wellcome to USpekPy!
- 2 How does USpekPy package work?
- 3 How to use USpekPy?
- 4 Wrapping up: What's next?

▶ Python usage poll

Wellcome to USpekPy!

- Wellcome to USpekPy!
 - What is USpekPy?
 - Main features of USpekPy
 - USpekPy in a nutshell
 - How to get support?
 - How to contribute to USpekPy?
- 2 How does USpekPy package work?
- 3 How to use USpekPy?
- 4 Wrapping up: What's next?



What is USpekPy?

- Python package: Open source and GPLv3-licensed library compatible with Python 3
- Goal: Compute mean radiation protection quantities for a simulated x-ray spectrum with uncertainties using Monte Carlo techniques
- Based on SpekPy: Python package for modelling the x-ray spectra from x-ray tubes

Main features of USpekPy

- Compute mean values of radiation protection quantities of a simulated x-ray spectrum: \overline{E} , K_{air} and $\overline{h_K}$
- Compute mean radiation protection quantities of a simulated x-ray spectrum with uncertainties using Monte Carlo techniques: first and second HVL for Al and Cu, \overline{E} , K_{air} and $\overline{h_K}$
- Perform batch simulation to compute mean values and uncertainties of radiation protection quantities for several simulated x-ray spectra

USpekPy in a nutshell

Status

1.0.2 Last version: Release date: Jun 2024 Maintenance: Active

Links

Source code: GitHub

README @GitHub Documentation:

Contribute: Issues @GitHub



Testing

Tests: Passing Code coverage: 65%

Distribution

Distribution: **PvPI**

GNU GPL v3.0

Requirements

Python: > 3.8Dependencies:

spekpy pandas

openpyxl

Authors

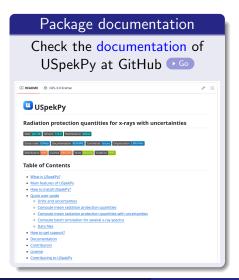
License:

Authors: X. Campo & P. Avilés Email: xandra.campo@ciemat.es

paz.aviles@ciemat.es

LMRI-Met @GitHub Organization:

How to get support?



Contact developers

Contact the developers of USpekPy via email:

Xandra Campo xandra.campo@ciemat.es

Paz Avilés paz.aviles@ciemat.es

How to contribute to USpekPy?

What may be a contribution?

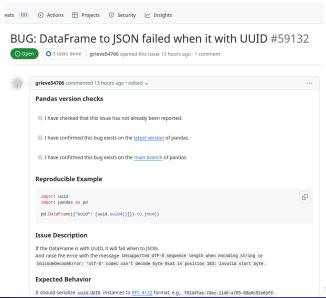
- Bug reports & fixes
- Documentation improvements
- Feature enhancements

How to deliver a contribution?

- Issues page at GitHub (Recommended)
- Contact the developers via email



What to include in a contribution?



Title

Description

Minimal.

Environment

Potential fix

Expected behavior

reproducible example

Error messages, logs

Steps to reproduce

How does USpekPy package work?

- Wellcome to USpekPy!
- 2 How does USpekPy package work?
 - Compute mean radiation protection quantities
 - Compute mean radiation protection quantities with uncertainties
 - Compute batch simulation for several x-ray spectra
 - Units and uncertainties convention
 - Verification of the code
- 3 How to use USpekPy?
- 4 Wrapping up: What's next?



Compute mean radiation protection quantities

Information flow

For a single case, given an x-ray quality and an operational quantity at a specific irradiation angle:

InputToolOutputValue:SpekWrapper classValue:• Filter thickness• HVL(AI, Cu)• Peak kilovoltage• \overline{E} • Anode angle• K_{air} • $h_K(E)$ • $\overline{h_K}$

Compute mean radiation protection quantities Workflow

Workflow for \overline{E} , K_{air} and $\overline{h_K}$:

- Compute x-ray spectrum (energy and fluence) using SpekPy
- ② If necessary, interpolate $\frac{\mu_{tr}}{\rho}(E)$ and $h_K(E)$ to spectrum energies in logarithmic scale
- If necessary, apply units conversion
- Compute the integral quantity using the corresponding definition

$$\overline{E} = \frac{\int_0^\infty \phi(E) E dE}{\int_0^\infty \phi(E) dE}$$

$$K_{air} = \int_0^\infty \phi(E) rac{\mu_{tr}}{
ho}(E) E dE$$

$$\overline{h_{K}} = \frac{\int_{0}^{\infty} \phi(E) \frac{\mu_{tr}}{\rho}(E) h_{K}(E) E dE}{\int_{0}^{\infty} \phi(E) \frac{\mu_{tr}}{\rho}(E) E dE}$$

HVLs are calculated using SpekPy methods.

4 D > 4 D > 4 E > 4 E > E 9 Q C

Compute mean RP quantities with uncertainties

Information flow

For a single case, given an x-ray quality and an operational quantity at a specific irradiation angle:

Input Tool Output **USpek class** Value and uncertainty: Value and uncertainty: Filter thickness HVL(Al, Cu) • F Peak kilovoltage Anode angle Kair \bullet $\overline{h_K}$ $\bullet \frac{\mu_{tr}}{\rho}(E)$ Value: \bullet $h_k(E)$

Number of iterations

Compute mean RP quantities with uncertainties Workflow

A simulation is performed for the specified number of iterations.

- For each iteration:
 - Generate random values of the input variables considering their mean values, uncertainties and distributions.
 - Compute mean values of the integral quantities using the SpekWrapper class
- Once the iterations are completed: Compute statistical mean value and standard deviation of the integral quantities from the different values obtained in the iterations

Compute batch simulation for several x-ray spectra

Information flow

For a set of cases, each case for a given x-ray quality and operational quantity at an irradiation angle:

Input

For every case:

Value and uncertainty:

- Filter thickness
- Peak kilovoltage
- Anode angle
- \bullet $\frac{\mu_{tr}}{\rho}(E)$

Value:

- h_k(E)
- Number of iterations

Tool

batch_simulation function

Output

For every case, value and uncertainty:

- HVL(AI, Cu)
- K_{air}
- ħ_K

Compute batch simulation for several x-ray spectra Workflow

- The set of cases are provided in an input file, each case is a column in that file
- 2 For each case, a simulation is performed for the specified number of iterations using the USpek class
- Results for the set of cases are returned in an output file, appending the result to the corresponding column of the input file

Units and uncertainties convention

- ullet All the uncertainties are standard uncertainties (k = 1)
- The units of relative uncertainties are expressed as fraction of one

Quantity	Unit
Distance	mm
Voltage	kV
Angle	deg
Energy	keV
Fluence	$1/cm^2$
Mass energy transfer coefficients of air	cm^2/g
Air kerma	μGy
Mono-energetic K to H conversion coefficients	Sv/Gy

Verification of the code

- Integral quantity values: Compared with values provided by SpekPy (except $\overline{h_K}$)
- Integral quantity uncertainties: Compared with values provided by:
 - Previous script version of USpekPy developed by Paz Avilés
 - Results obtained by CMI

How to use USpekPy?

- Wellcome to USpekPy!
- 2 How does USpekPy package work?
- 3 How to use USpekPy?
 - How to install USpekPy?
- Wrapping up: What's next?

How to install USpekPy?

Prerequisites

1. Prerequisites

- Make sure you have Python installed.
- USpekPy requires Pyhton 3.8 or superior.
- To check the Python version use the next command on your OS terminal:

```
$ python3 --version
```

How to install USpekPy?

Virtual environment

2. Set up a virtual environment

Virtual environment: Tool built into Python that provides isolated Python environments, which are more practical than installing packages systemwide. It allows to keep a separate directory of installed packages for each of your projects so that they don't interfere with each other. Navigate to the directory where you're Python project will live.

→ロト→部ト→差ト→差 のQで

How to install USpekPy?

Install USpekPy

3. Install USpekPy

\$ pip install uspekpy

Wrapping up: What's next?

- Wellcome to USpekPy!
- 2 How does USpekPy package work?
- 3 How to use USpekPy?
- Wrapping up: What's next?
 - Improvements on the horizon
 - Let us know what you think

Improvements on the horizon

- Bug: Fix SciPy dependency bug
- New feature: Add the contribution to the uncertainty of the variation of the mono-energetic air kerma-to-dose conversion coefficients
- Documentation: Improve package documentation (GitHub Wiki, GitHub Pages)
- Testing: Improve test code coverage

Let us know what you think

Complete our satisfaction survey about this seminar! Help us make future seminars better.

➤ Satisfaction survey

Contribute to USpekPy package!

This sofware is for you. We want to make it fit better your necesities. Let us know if you find any issue or if you would like to have any new feature in future versions.

▶ USpekPy Issues page

xandra.campo@ciemat.es paz.aviles@ciemat.es



Thank you very much!

We're grateful for your time and attention today.

We appreciate your interest in USpekPy.

Thank you for joining us.