

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

- 1 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!

- 1 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 [▶ Go](#)
- **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 [▶ Go](#)

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

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

Links

Source code: [GitHub](#)
Documentation: [README @GitHub](#)
Contribute: [Issues @GitHub](#)

[▶ Go](#)[▶ Go](#)[▶ Go](#)

Testing

Tests: Passing
Code coverage: 65%

Distribution

Distribution: [PyPI](#)
License: [GNU GPL v3.0](#)

[▶ Go](#)[▶ Go](#)

Requirements

Python: ≥ 3.8
Dependencies: spekpy
pandas
openpyxl

Authors

Authors: X. Campo & P. Avilés
Email: xandra.campo@ciemat.es
paz.aviles@ciemat.es
Organization: [LMRI-Met @GitHub](#)

[▶ Go](#)

How to get support?

Package documentation

Check the [documentation](#) of
USpekPy at GitHub [► Go](#)

The screenshot shows the GitHub README for the USpekPy package. At the top, it says 'USpekPy' with a logo. Below that, it states 'Radiation protection quantities for x-rays with uncertainties'. There are badges for 'Date: Jan 24', 'Version: 1.0.2', and 'Maintenance: Active'. A row of links includes 'Source code', 'Documentation', 'README', 'Contribute', 'Issues', 'Organization', and 'Links'. Another row includes 'Distributions', 'PyPI', 'License', 'SPDX', 'Tests', 'Badges', 'Codecov', and 'Docs'. A 'Table of Contents' section lists links for 'What is USpekPy?', 'Main features of USpekPy', 'How to install USpekPy?', 'Quick user guide' (with sub-links for 'Units and uncertainties', 'Compute mean radiation protection quantities', 'Compute mean radiation protection quantities with uncertainties', 'Compute batch simulation for several x-ray spectra', and 'Data files'), 'How to get support?', 'Documentation', 'Contributors', 'License', and 'Contributing to USpekPy'.

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) [▶ Go](#)
- Contact the developers [via email](#)

<input type="checkbox"/>	1 Open ✓ 7 Closed	Author ▾	Label ▾	Projects ▾	Milestones ▾	Assignee ▾	Sort ▾
<input type="checkbox"/>	🟢 Using the latest stable SciPy release (version 1.14.0) will cause USpekPy to crash bug #9 opened yesterday by pazaviles						
<input type="checkbox"/>	🟢 Value of kerma miscalculated bug #8 by xandratxan was closed last week						1
<input type="checkbox"/>	🟢 Batch simulation can't proceses 4 or more simulation cases bug #6 by xandratxan was closed 2 weeks ago				1		

What to include in a contribution?

- Title
- Description
- Expected behavior
- Steps to reproduce
- Minimal, reproducible example
- Environment
- Error messages, logs
- Potential fix

ests 101 Actions Projects Security Insights

BUG: DataFrame to JSON failed when it with UUID #59132

Open 3 tasks done griev54706 opened this issue 13 hours ago · 1 comment

griev54706 commented 13 hours ago · edited

Pandas version checks

- ☒ I have checked that this issue has not already been reported.
- ☒ I have confirmed this bug exists on the [latest version](#) of pandas.
- ☒ I have confirmed this bug exists on the [main branch](#) of pandas.

Reproducible Example

```
import uuid
import pandas as pd

pd.DataFrame({"uuid": [uuid.uuid4()]}) .to_json()
```

Issue Description

If the DataFrame is with UUID, it will fail when to JSON.
And raise the error with the message: `Unsupported UTF-8 sequence length when encoding string` or `UnicodeDecodeError: 'utf-8' codec can't decode byte 0xa1 in position 183: invalid start byte`.

Expected Behavior

It should serialize `uuid.UUID` instances to [RFC 4122](#) format, e.g., `f81d4fae-7dec-11d0-a765-00a0c91e6bf6`.

How does USpekPy package work?

1 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:

Input

Value:

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

Tool

SpekWrapper class

Output

Value:

- $HVL(Al, Cu)$
- \bar{E}
- K_{air}
- \bar{h}_K

Compute mean radiation protection quantities

Workflow

Workflow for \bar{E} , K_{air} and \bar{h}_K :

- ① 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
- ③ If necessary, apply **units** conversion
- ④ Compute the **integral quantity** using the corresponding definition

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

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

$$\bar{h}_K = \frac{\int_0^\infty \phi(E) \frac{\mu_{tr}}{\rho}(E) h_K(E) E dE}{\int_0^\infty \phi(E) \frac{\mu_{tr}}{\rho}(E) E dE}$$

HVLs are calculated using SpekPy methods.

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

Value and uncertainty:

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

Value:

- $h_k(E)$
- Number of iterations

Tool

USpek class

Output

Value and uncertainty:

- HVL(Al, Cu)
- \bar{E}
- K_{air}
- \bar{h}_K

Compute mean RP quantities with uncertainties

Workflow

A simulation is performed for the specified number of iterations.

① For each iteration:

- ① **Generate random values** of the input variables considering their mean values, uncertainties and distributions.
- ② **Compute mean values** of the integral quantities using the SpekWrapper class

② 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
- $\frac{\mu_{tr}}{\rho}(E)$

Value:

- $h_k(E)$
- Number of iterations

Tool

`batch_simulation`
function

Output

For every case,
value and uncertainty:

- $HVL(Al, Cu)$
- \bar{E}
- K_{air}
- $\bar{h_K}$

Compute batch simulation for several x-ray spectra

Workflow

- 1 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
- 3 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

- 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	$1/\text{cm}^2$
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?

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

How to install USpekPy?

Prerequisites

1. Prerequisites

- Make sure you have [Python](#) installed.
- USpekPy requires Python 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.

How to install USpekPy?

Install USpekPy

3. Install USpekPy

```
$ pip install uspekpy
```

Wrapping up: What's next?

- 1 Wellcome to USpekPy!
- 2 How does USpekPy package work?
- 3 How to use USpekPy?
- 4 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 software is for you. We want to make it fit better your necessities. 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.