

# 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?

# 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](#)

[▶ Python usage poll](#)

# 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:  $\geq 3.8$   
Dependencies: spekpy  
pandas  
openpyxl

## Authors

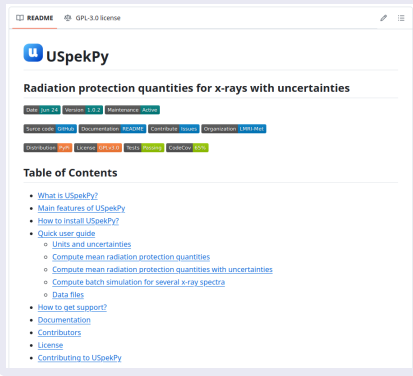
Authors: X. Campo & P. Avilés  
Email: [xandra.campo@ciemat.es](mailto:xandra.campo@ciemat.es)  
[paz.aviles@ciemat.es](mailto:paz.aviles@ciemat.es)  
Organization: [LMRI-Met @GitHub](#)

[▶ 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, there's a 'README' tab and a 'GPL-3.0 license' indicator. The USpekPy logo is prominently displayed. Below it, the title 'Radiation protection quantities for x-rays with uncertainties' is shown. A metadata bar includes 'Date: Jan 24', 'Version: 1.0.2', and 'Maintenance: Active'. Navigation links for 'Source code', 'Documentation', 'README', 'Contribute', 'Issues', 'Organization', and 'Links' are provided. A secondary row of links includes 'Distributions', 'PyPI', 'License', 'SPDX', 'Tests', 'Building', and 'Codecov'. A 'Table of Contents' section lists various links: '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](mailto:xandra.campo@ciemat.es)

Paz Avilés  
[paz.aviles@ciemat.es](mailto: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"/>	🟢 <b>Using the latest stable SciPy release (version 1.14.0) will cause USpekPy to crash</b> <span>bug</span>						
	#9 opened yesterday by pazaviles						
<input type="checkbox"/>	🟢 <b>Value of kerma miscalculated</b> <span>bug</span>						1
	#8 by xandratxan was closed last week						
<input type="checkbox"/>	🟢 <b>Batch simulation can't proceses 4 or more simulation cases</b> <span>bug</span>						1
	#6 by xandratxan was closed 2 weeks ago						



# What to include in a contribution?

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

The screenshot shows a GitHub issue page for the project 'USpekPy'. The issue title is 'BUG: DataFrame to JSON failed when it with UUID #59132'. It has 3 tasks done and was opened 13 hours ago by user 'grieve54706'. The issue content includes a section for 'Pandas version checks' with three checked items: 'I have checked that this issue has not already been reported.', 'I have confirmed this bug exists on the latest version of pandas.', and 'I have confirmed this bug exists on the main branch of pandas.'. There is a 'Reproducible Example' section with a code block showing the following Python code: 

```
import uuid
import pandas as pd

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

. The 'Issue Description' section states: '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.'. The 'Expected Behavior' section states: 'It should serialize uuid.UUID instances to RFC4122 format, e.g., f81d4fae-7dec-11d0-a765-00a0c91e6bf6.'.

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 [RFC4122](#) 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	$\text{cm}^2/\text{g}$
Air kerma	$\mu\text{Gy}$
Mono-energetic K to H conversion coefficients	$\text{Sv/Gy}$

# 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?
- 4 Wrapping up: What's next?

# 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.