

# Uncertainty quantification of depletion calculations for specific isotopes using ORIGEN2

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**NUCLEAR SECURITY  
SCIENCE & POLICY INSTITUTE**

# Outline

## Background

- Introduction

- Current Problem

## Objectives

- ORIGEN2 Model

- Cross Section Variations

- Variance for cross-sections

- Sampling Space and Plotting Program

## Results

## Conclusions

- ❖ Determining composition of irradiated fuel importance
  - Flux calculations
  - Reprocessing
  - Irradiation history verification
- ❖ Usually determined with a type of Bateman solver
- ❖ Uncertainties rarely reported
  - Flux Shape
  - Fission yield
  - **Cross Sections**
  - Half-lives

- ❖ Use of depletion code ORIGEN2
  - Solves with exponential method
  - Requires libraries
    - ◆ Decay information
    - ◆ Fission yield data
    - ◆ Single group cross sections
- ❖ PWR system with 3 wt% enriched uranium
- ❖ Varied  $\sigma_\gamma$  and  $\sigma_f$  for:  $^{235}\text{U}$ ,  $^{238}\text{U}$ ,  $^{239}\text{Pu}$ ,  $^{240}\text{Pu}$ , and  $^{241}\text{Pu}$ 
  - Originally,  $\sigma_\gamma$  and  $\gamma$  for the FP were considered

## Quantities of Interest

$^{133}\text{Cs}$	$^{136}\text{Ba}$	$^{153}\text{Eu}$
$^{134}\text{Cs}$	$^{138}\text{Ba}$	$^{154}\text{Eu}$
$^{135}\text{Cs}$	$^{149}\text{Sm}$	$^{239}\text{Pu}$
$^{137}\text{Cs}$	$^{150}\text{Sm}$	$^{242}\text{Pu}$
$^{148}\text{Nd}$	$^{106}\text{Rh}$	$^{125}\text{Sb}$

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- ❖ Model irradiates 1 metric ton of US PWR fuel for a single cycle (15,000 MWd/Mt)
- ❖ Constant power assumption (37.5 W/g)
- ❖ Does not include oxygen
- ❖ Verified with  $^{137}\text{Cs}$  content

$$\frac{552.8 \text{ g } ^{137}\text{Cs}}{\text{Mt}} \cdot \frac{6.022E23 \text{ atoms}}{137 \text{ g } ^{137}\text{Cs}} \cdot \frac{\text{Fission}}{0.06 \text{ atoms}} \cdot \frac{200 \text{ MeV}}{\text{Fission}} \cdot \frac{1.602E-19 \text{ MJ}}{1 \text{ MeV}} \cdot \frac{1 \text{ day}}{86400 \text{ s}} = 15,018 \frac{\text{MWd}}{\text{Mt}}$$

# ORIGEN2 Model

```

RDA  Irradiation of 1 MT of PWR fuel
RDA  Fuel enrichment is 3.0 w/o U-235
RDA
LPU  922350  922380  942390  942400  942410
5  LIB  0   1  2  3   601 -602  603   9   8  0  1  38
   PHO      101 102 103   10
   INP  1   1  -1  -1   1   1
   BUP
10  IRP 100.0 37.5 1 2 4 2 BURNUP=3,750 MMD/MT
   IRP 200.0 37.5 2 3 4 0 BURNUP=7,500 MMD/MT
   IRP 300.0 37.5 3 4 4 0 BURNUP=11,250 MMD/MT
   IRP 400.0 37.5 4 5 4 0 BURNUP=15,000 MMD/MT
   DEC 500.0      5 6 4 0 DECAY FOR 100.0 DAYS
   DEC 4150.0     6 7 4 0 DECAY FOR 10 YEARS
15  DEC 73500.0    7 8 4 0 DECAY FOR 200.0 YEARS
   BUP
   OPTL 24*8
   OPTA 4*8 5 19*8
   OPTF 4*8 5 19*8
20  OUT      8   1  -1   0
   END
2  922340 270. 922350 30000. 922380 969730. 0 0.0
```

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# How the manual says it is\*...

- ❖ TAPE9.inp (8th input on LIB card)
- ❖ TAPE8.inp (9th input on LIB card)
  - Sorry for the confusion
- ❖ LPU card
  - Short for Lost Plutonium\*
- ❖ Programed both, neither worked
  - The first lied to my face
  - The second complained about: “An endfile record was detected in a READ statement (unit= 8)”
  - Didn't find out about the lying until last night

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LIB	NUCLID	(n, $\gamma$ )	(n,2n)	(n,3n)	(n,f)	(n, $\gamma^*$ )	(n,2n <sup>*</sup> )	YYN
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\* Its not Really

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# Cross-section calculations

$$\sigma = \frac{\int \sigma(E) \phi(E) dE}{\int \phi(E) dE}$$

$$\phi(E) = C_1 \cdot \frac{E}{E_0^2} \cdot \exp\left(-\frac{E}{E_0}\right) \quad E < E_{max,th}$$

$$= \frac{C_2}{E} \quad E_{max,th} < E < E_{max,epi}$$

$$= C_3 \cdot \frac{\sqrt{\frac{E}{E_f}}}{E_f} \cdot \exp\left(-\frac{E}{E_f}\right) \quad E > E_{max,epi}$$

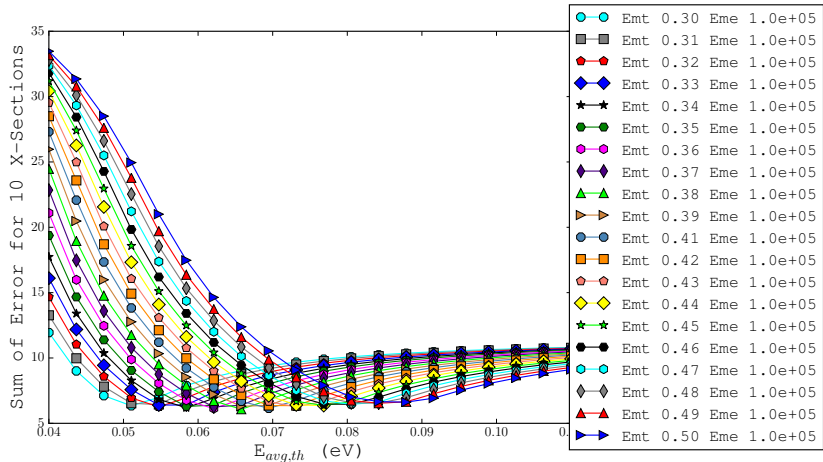
$$C_1 = \frac{E_0^2}{E_{max,th}^2} e^{E_{max,th}/E_0}$$

$$C_2 = 1$$

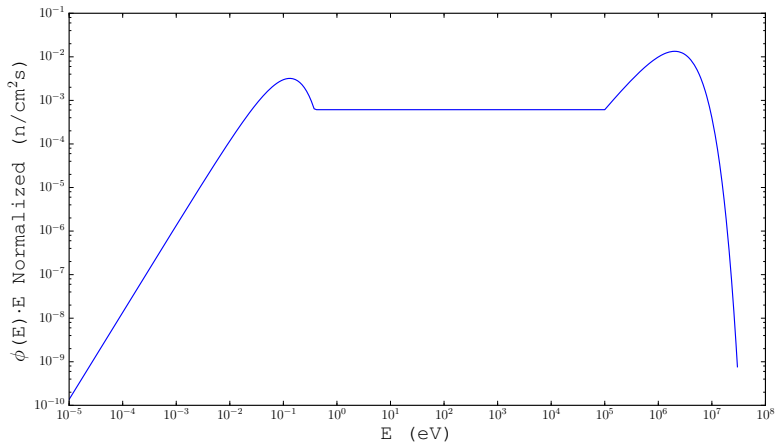
$$C_3 = \frac{E_f}{E_{max,epi}} \cdot e^{\frac{E_{max,epi}}{E_f}} \frac{1}{\sqrt{\frac{E_{max,epi}}{E_f}}}$$

$$E_{max,th} = 0.50 \text{ eV}, E_{max,epi} = 1E5 \text{ eV}, \theta_{th} = 0.09 \text{ eV (764 K)}, \theta_{fis} = 1.35E6 \text{ eV}$$

# Difference Minimization

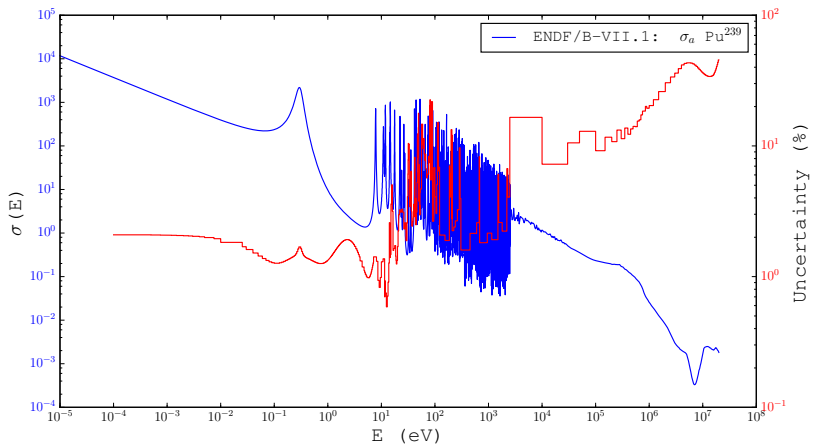


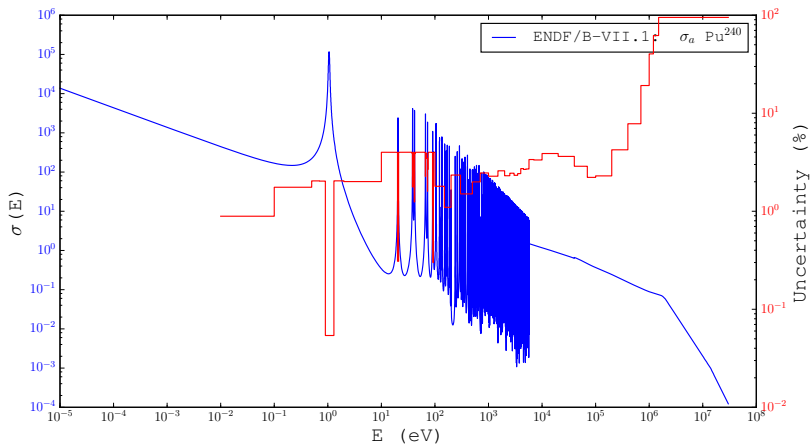
# Flux Distribution



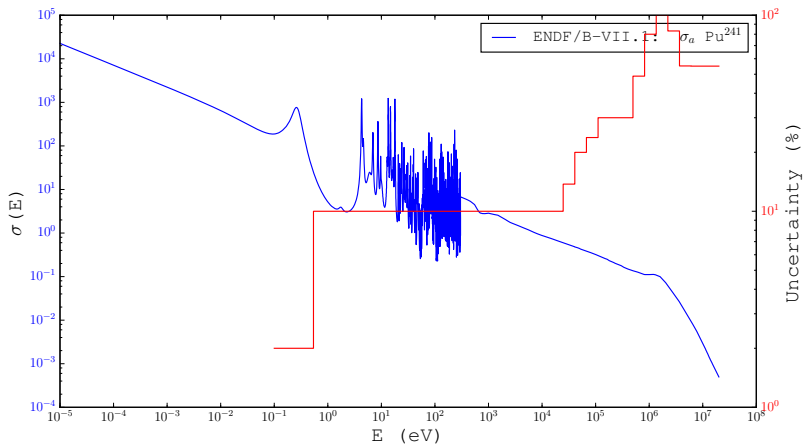
# One Group Cross Section Comparison

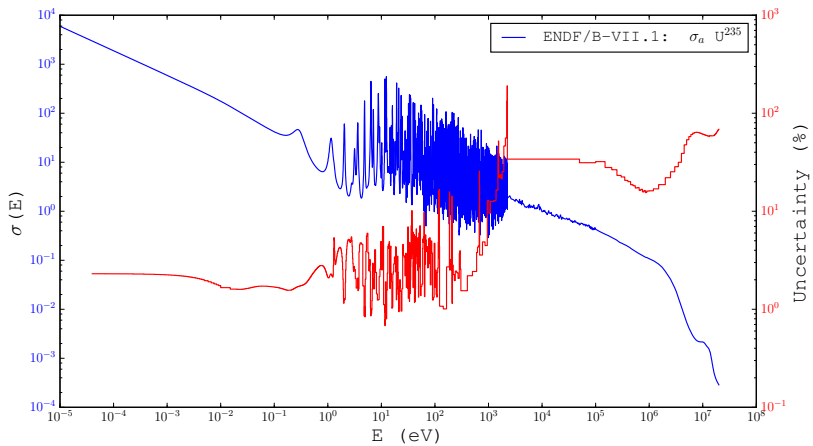
Isotope <sup>Rxn</sup>	ENDF VII	ORIGEN2	Ratio
<sup>239</sup> Pu <sup>γ</sup>	6.544e+01	6.909E+01	1.06
<sup>240</sup> Pu <sup>γ</sup>	1.521e+02	2.228E+02	1.46
<sup>241</sup> Pu <sup>γ</sup>	4.518e+01	4.202E+01	0.93
<sup>235</sup> U <sup>γ</sup>	9.387e+00	1.068E+01	1.14
<sup>238</sup> U <sup>γ</sup>	4.098e+00	8.872E-01	0.22
<sup>239</sup> Pu <sup>f</sup>	1.179e+02	1.211E+02	1.03
<sup>240</sup> Pu <sup>f</sup>	9.609e-01	5.787E-01	0.60
<sup>241</sup> Pu <sup>f</sup>	1.253e+02	1.259E+02	1.01
<sup>235</sup> U <sup>f</sup>	4.621e+01	4.752E+01	1.03
<sup>238</sup> U <sup>f</sup>	2.091e-01	9.281E-02	0.44

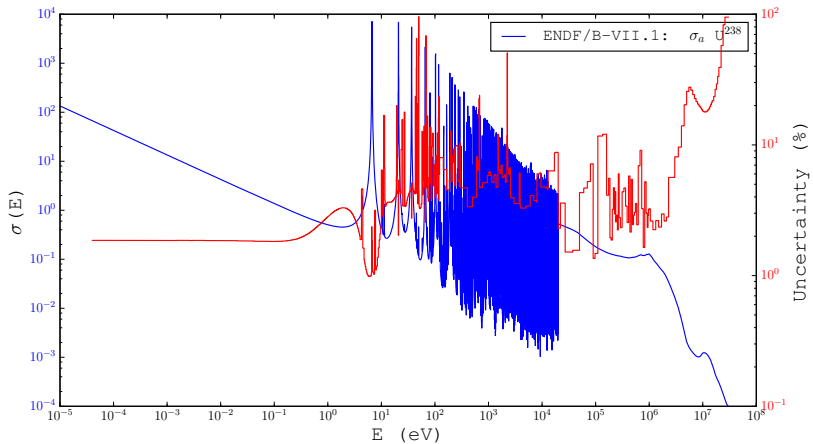


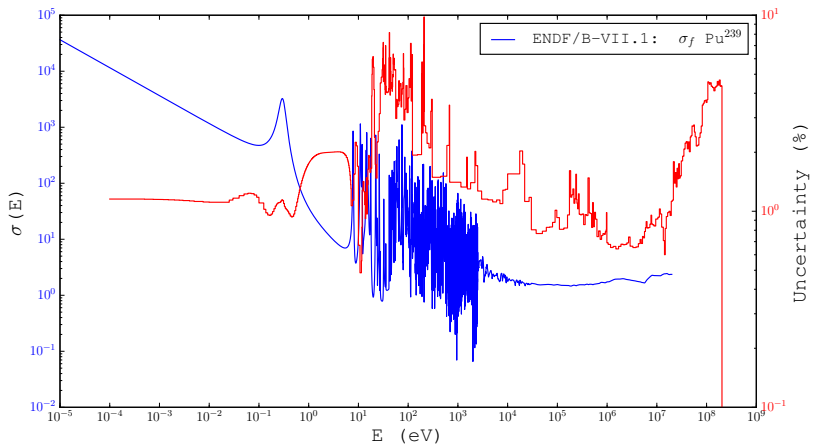


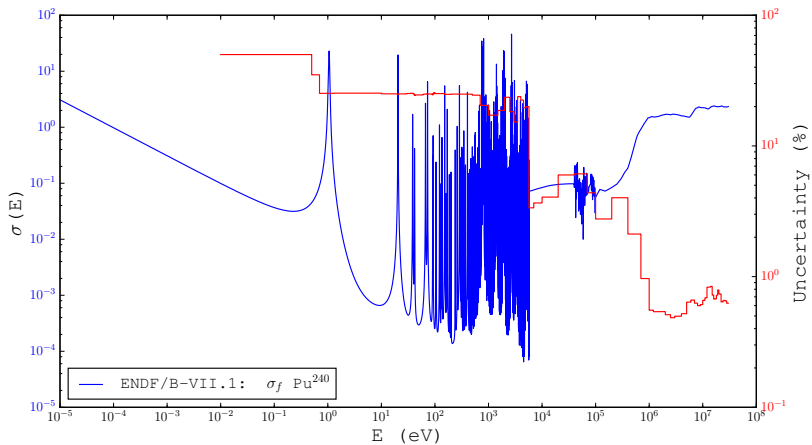


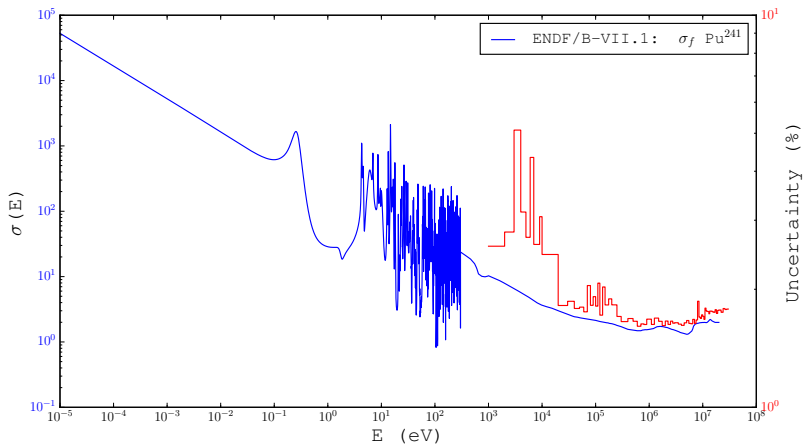


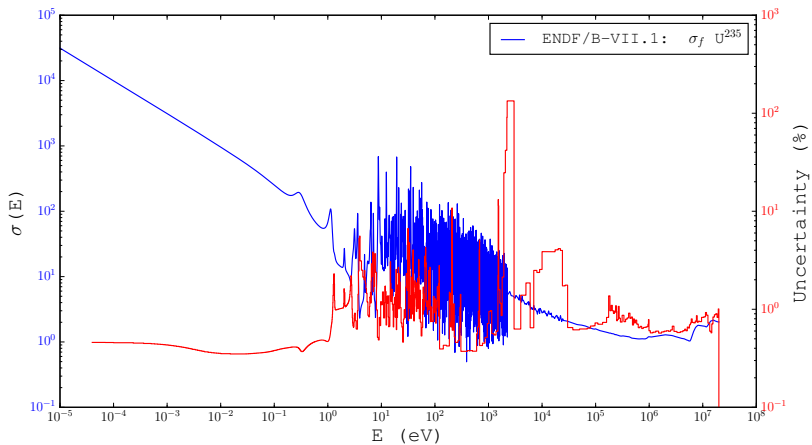


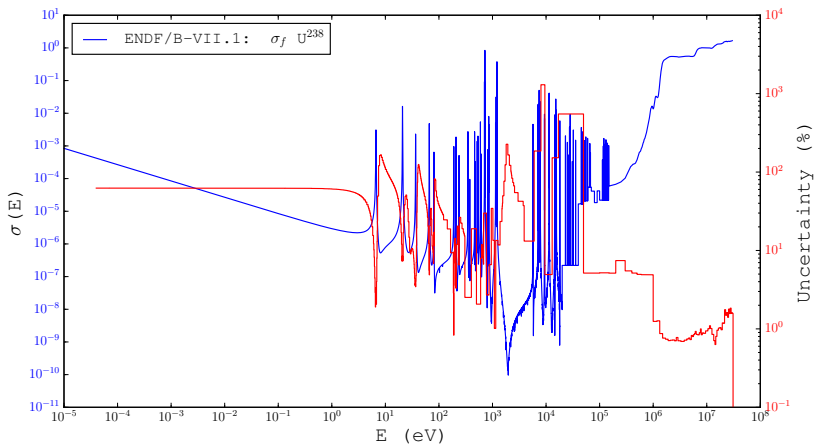














# Single Group Cross Sections with Errors

Isotope <sup>Rxn</sup>	$\sigma$ with 1STD Error
<sup>239</sup> Pu $\gamma$	69.09 $\pm$ 8.15
<sup>240</sup> Pu $\gamma$	222.8 $\pm$ 50.9
<sup>241</sup> Pu $\gamma$	42.02 $\pm$ 10.92
<sup>235</sup> U $\gamma$	10.68 $\pm$ 3.23
<sup>238</sup> U $\gamma$	0.887 $\pm$ 0.175
<sup>239</sup> Pu <sup>f</sup>	121.1 $\pm$ 1.2
<sup>240</sup> Pu <sup>f</sup>	0.579 $\pm$ 0.003
<sup>241</sup> Pu <sup>f</sup>	125.9 $\pm$ 2.3
<sup>235</sup> U <sup>f</sup>	47.52 $\pm$ 0.71
<sup>238</sup> U <sup>f</sup>	0.093 $\pm$ 8.2e-7

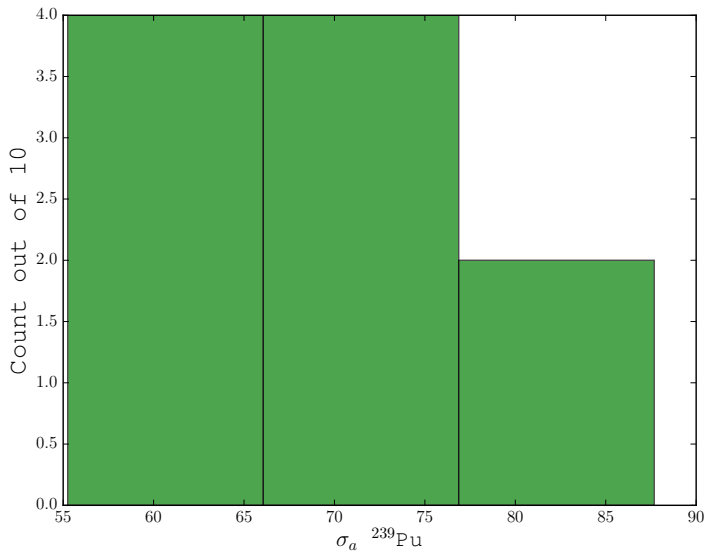
## Objectives

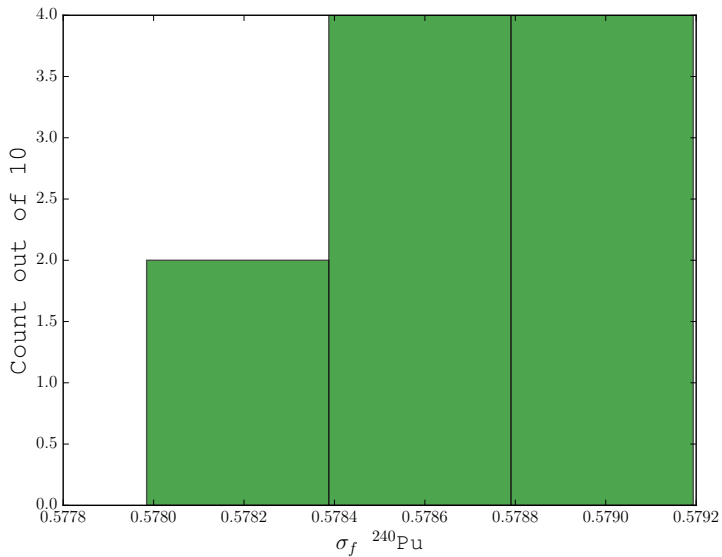
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$$\pi(\theta) = \frac{\theta^{\alpha-1} e^{-\theta/\beta}}{\Gamma(\alpha) \beta^\alpha}, \quad \theta, \alpha, \beta > 0.$$

$$\alpha = \frac{\text{Mean}^2}{\text{Error}^2}$$

$$\beta = \frac{\text{Error}^2}{\text{Mean}}$$

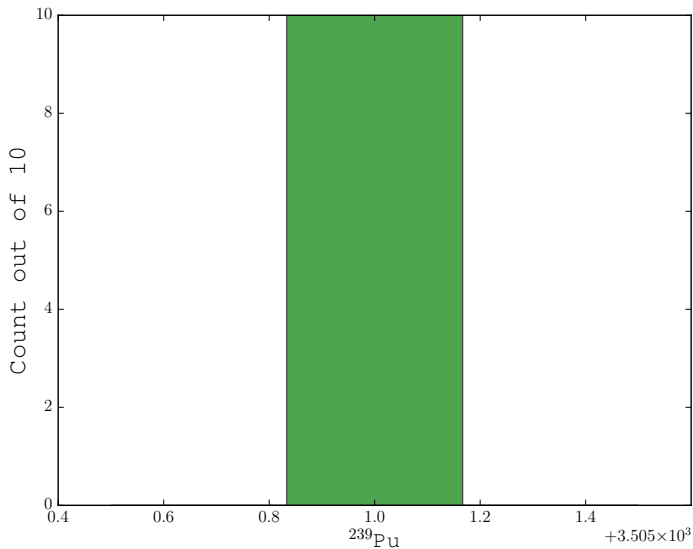




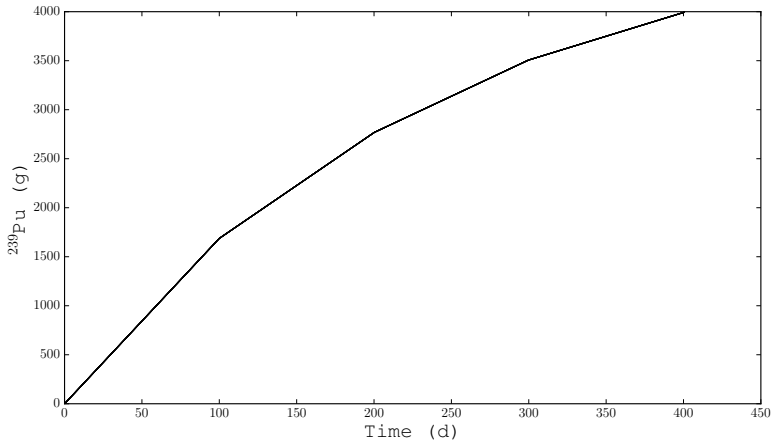
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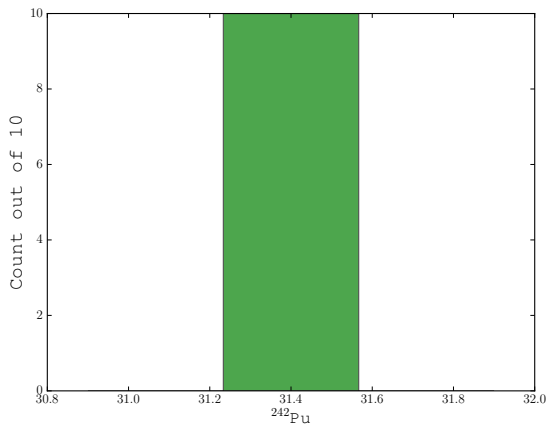
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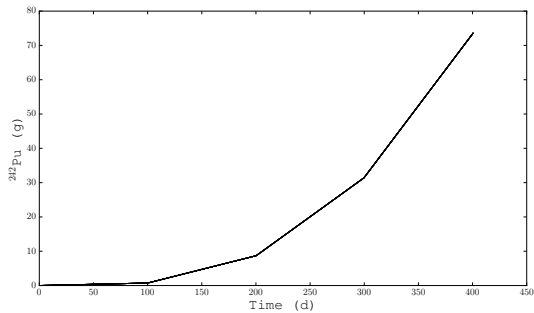
# Results

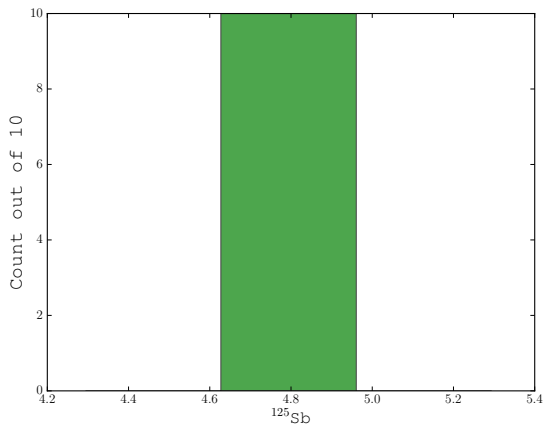


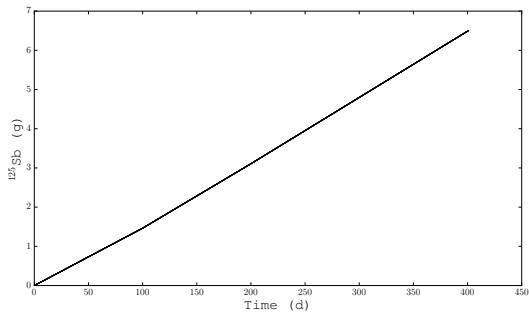


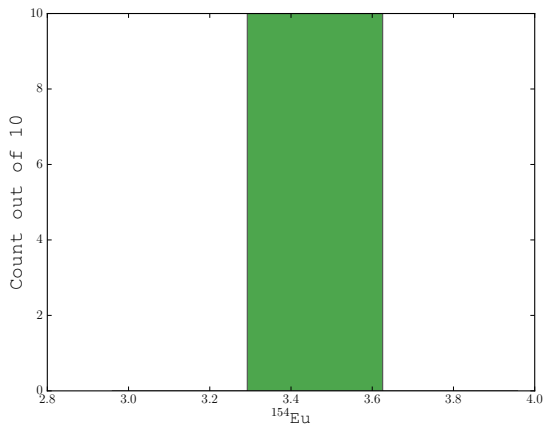


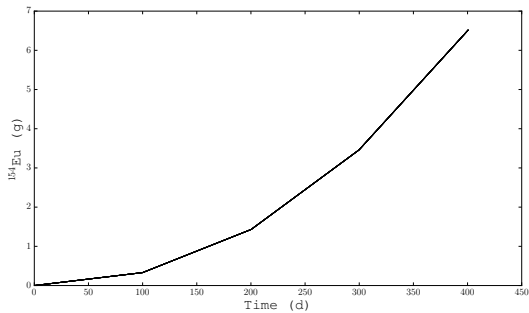


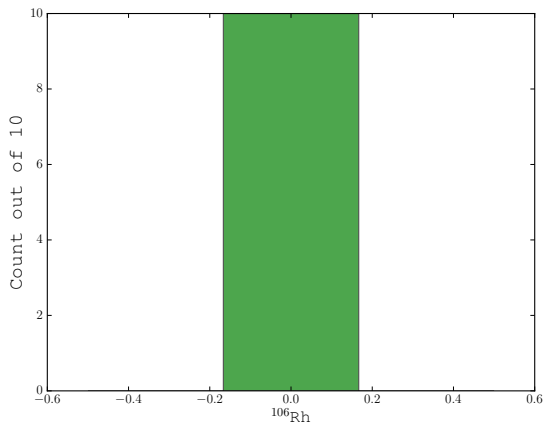




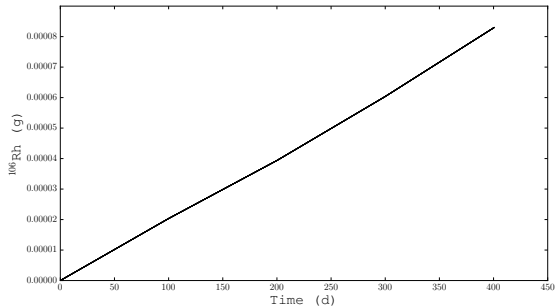


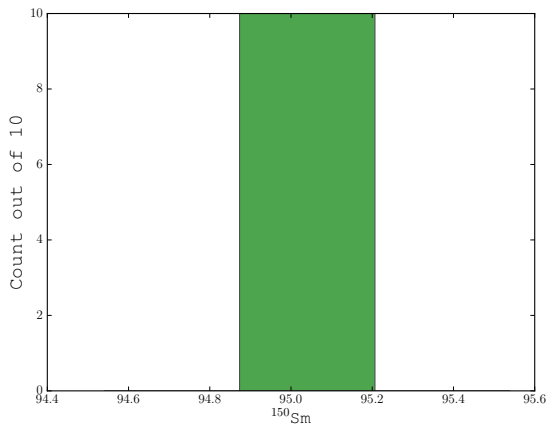


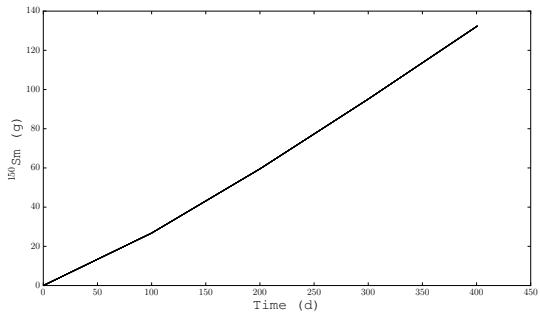


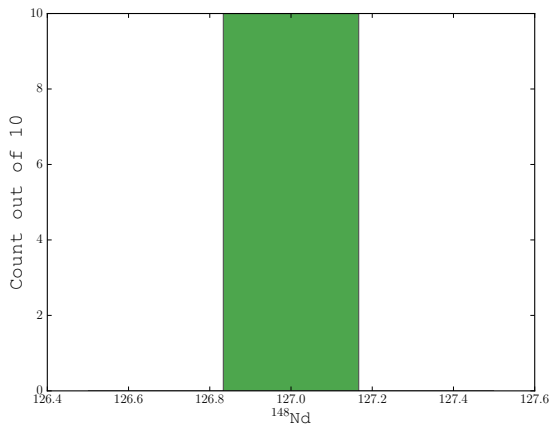


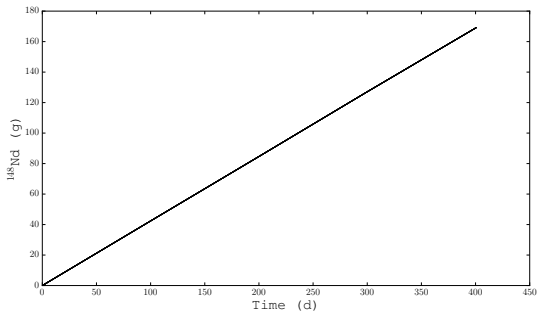


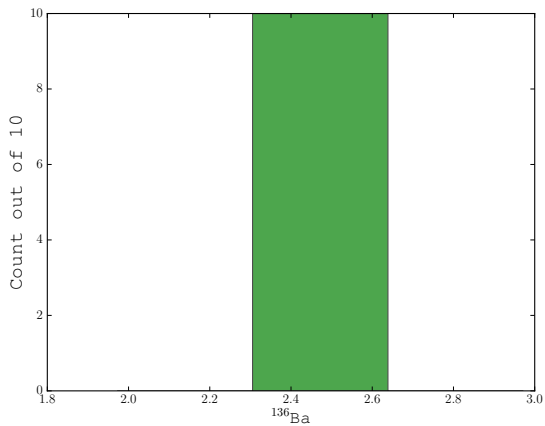


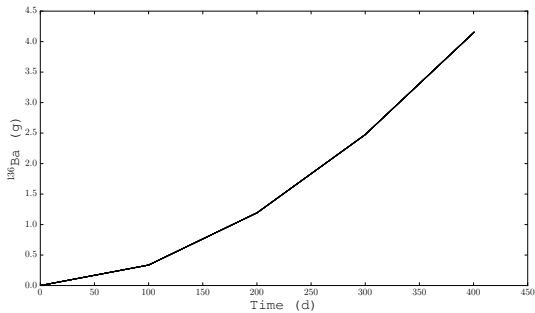


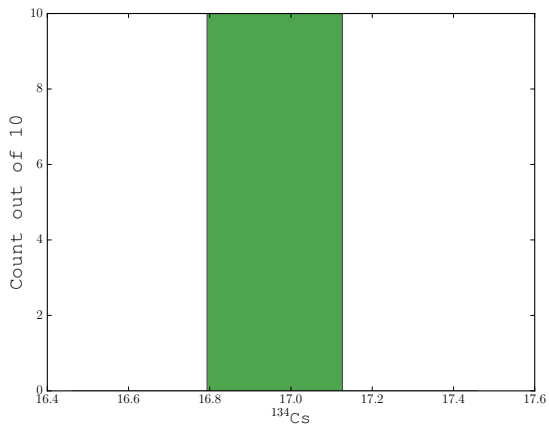




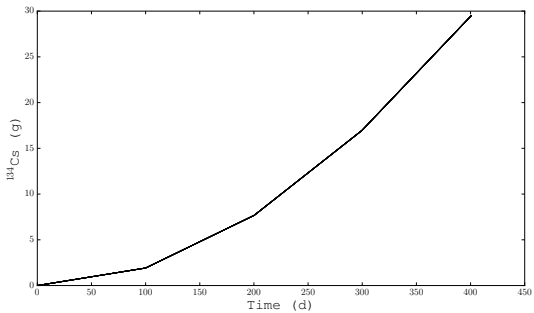












# Conclusions

- ❖ Surprised at size of error
- ❖ Sad it didn't work fully

