

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 σ_γ and σ_f for: ^{235}U , ^{238}U , ^{239}Pu , ^{240}Pu , and ^{241}Pu
 - Originally, σ_γ and γ for the FP were considered

Quantities of Interest

^{133}Cs	^{136}Ba	^{153}Eu
^{134}Cs	^{138}Ba	^{154}Eu
^{135}Cs	^{149}Sm	^{239}Pu
^{137}Cs	^{150}Sm	^{242}Pu
^{148}Nd	^{106}Rh	^{125}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}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  -1
5  LIB  1  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

LIB	NUCLID	(n, γ)	(n,2n)	(n,3n)	(n,f)	(n, γ^*)	(n,2n [*])	YYN
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* Its not Really

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Cross-section calculations

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

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

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

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

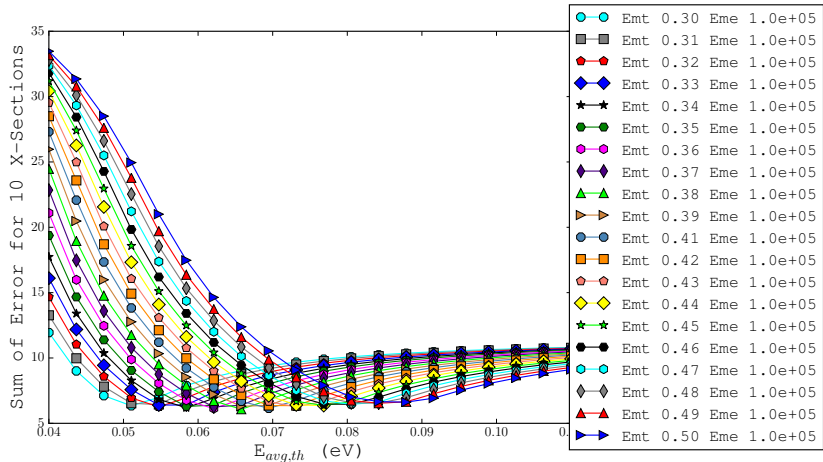
$$C_1 = \frac{E_0^2}{E_{max,th}^2} e^{E_{max,th}/E_0}$$

$$C_2 = 1$$

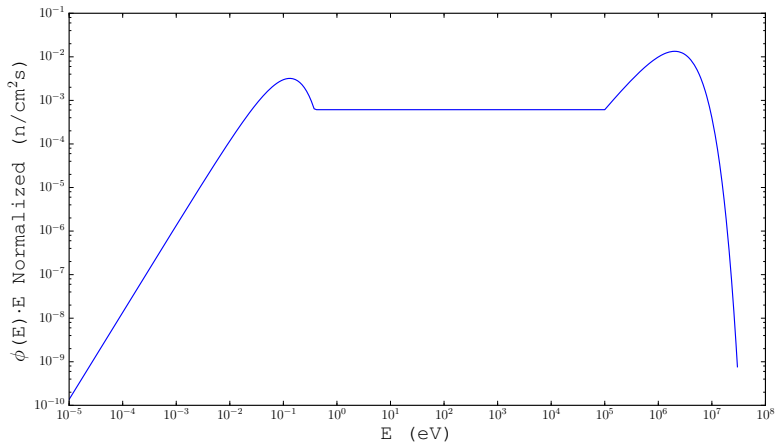
$$C_3 = \frac{E_f}{E_{max,epi}} \cdot e^{\frac{E_{max,epi}}{E_f}} \frac{1}{\sqrt{\frac{E_{max,epi}}{E_f}}}$$

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

Difference Minimization

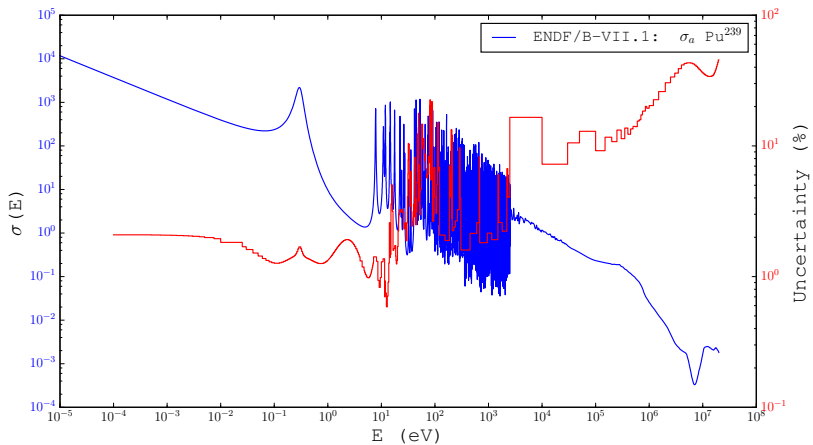


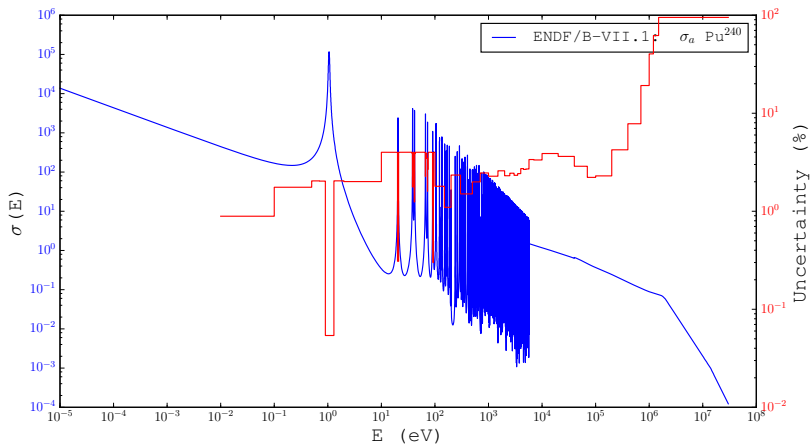
Flux Distribution

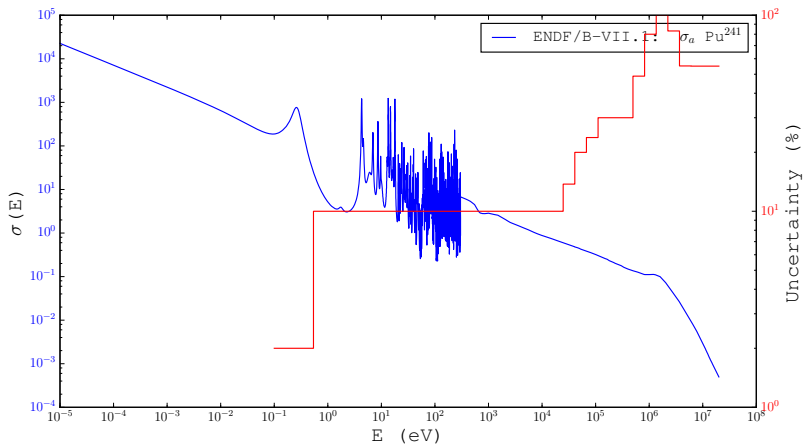


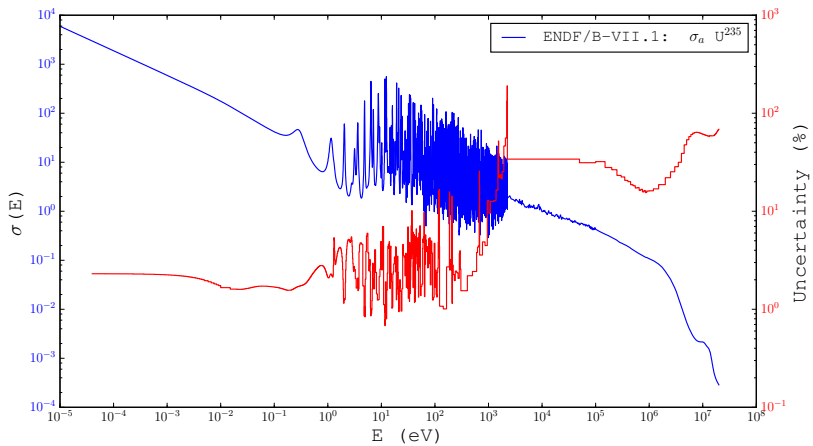
One Group Cross Section Comparison

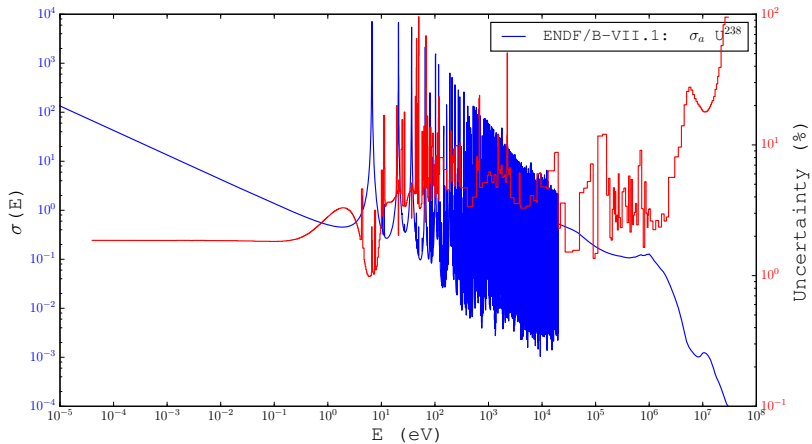
Isotope ^{Rxn}	ENDF VII	ORIGEN2	Ratio
²³⁹ Pu ^γ	6.544e+01	6.909E+01	1.06
²⁴⁰ Pu ^γ	1.521e+02	2.228E+02	1.46
²⁴¹ Pu ^γ	4.518e+01	4.202E+01	0.93
²³⁵ U ^γ	9.387e+00	1.068E+01	1.14
²³⁸ U ^γ	4.098e+00	8.872E-01	0.22
²³⁹ Pu ^f	1.179e+02	1.211E+02	1.03
²⁴⁰ Pu ^f	9.609e-01	5.787E-01	0.60
²⁴¹ Pu ^f	1.253e+02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

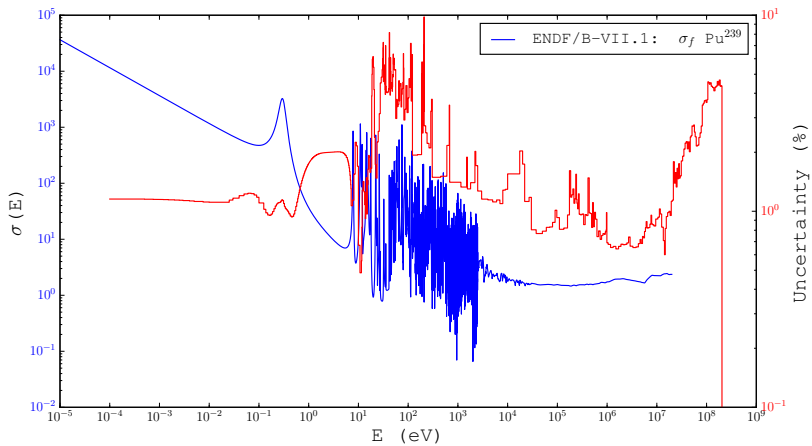


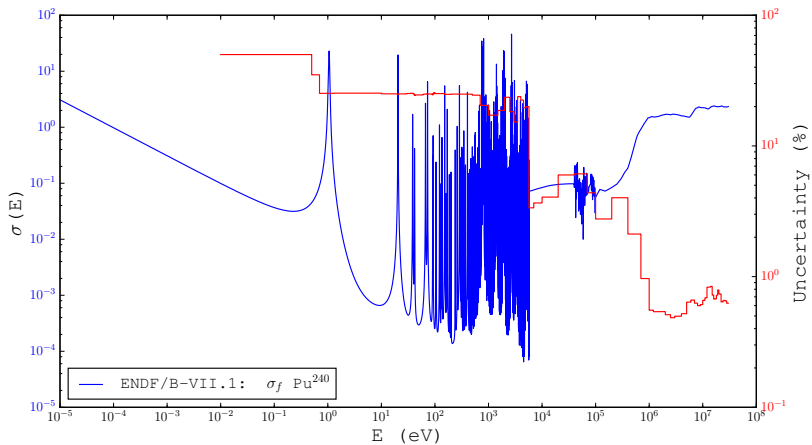


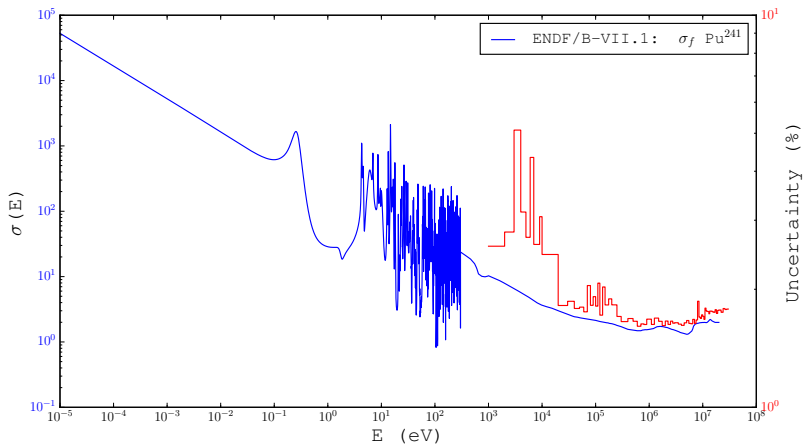


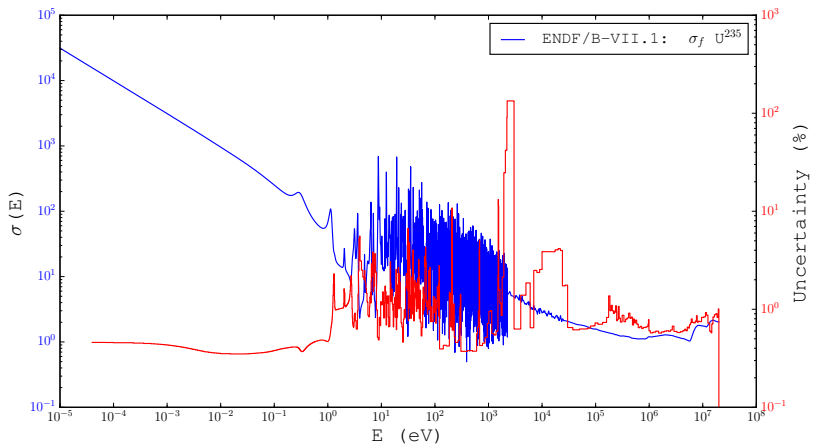


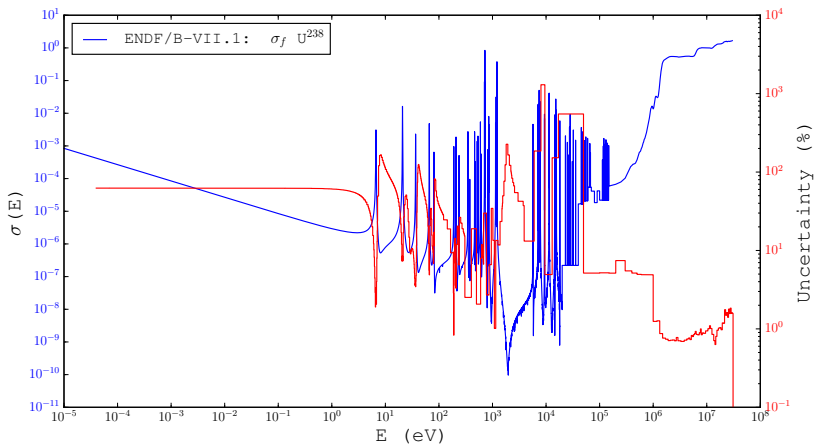












Single Group Cross Sections with Errors

Isotope ^{Rxn}	σ with 1STD Error
²³⁹ Pu γ	69.09 \pm 8.15
²⁴⁰ Pu γ	222.8 \pm 50.9
²⁴¹ Pu γ	42.02 \pm 10.92
²³⁵ U γ	10.68 \pm 3.23
²³⁸ U γ	0.887 \pm 0.175
²³⁹ Pu ^f	121.1 \pm 1.2
²⁴⁰ Pu ^f	0.579 \pm 0.003
²⁴¹ Pu ^f	125.9 \pm 2.3
²³⁵ U ^f	47.52 \pm 0.71
²³⁸ U ^f	0.093 \pm 8.2e-7

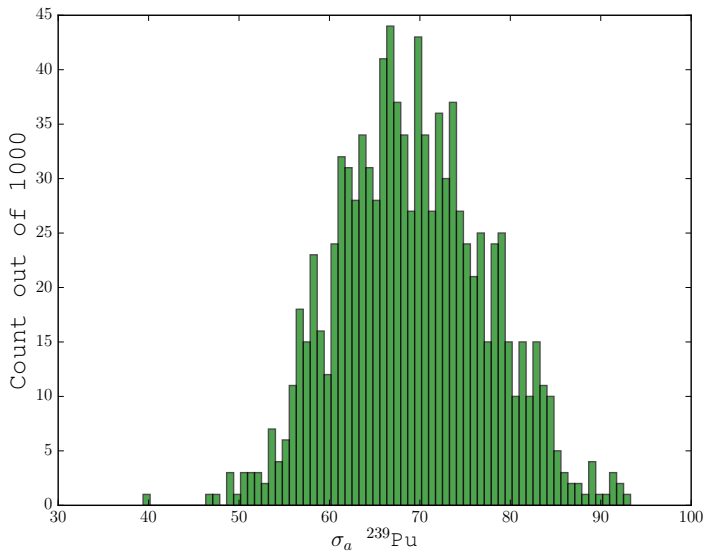
Objectives

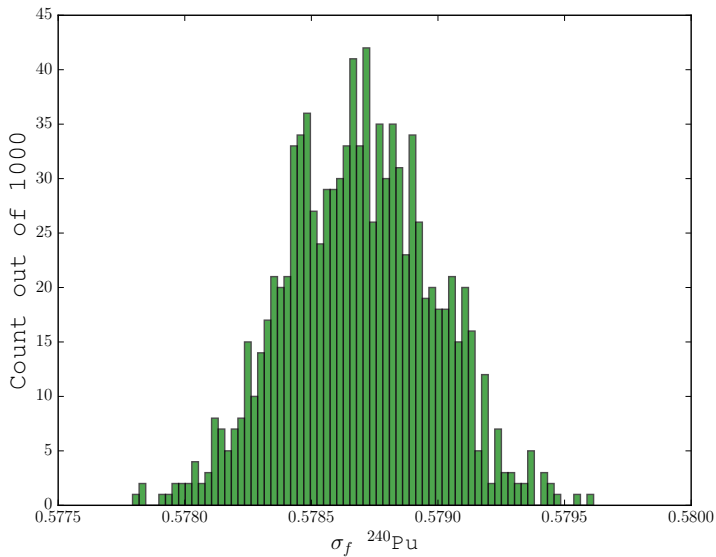
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$$\pi(\theta) = \frac{\theta^{\alpha-1} e^{-\theta/\beta}}{\Gamma(\alpha) \beta^\alpha}, \quad \theta, \alpha, \beta > 0.$$

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

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

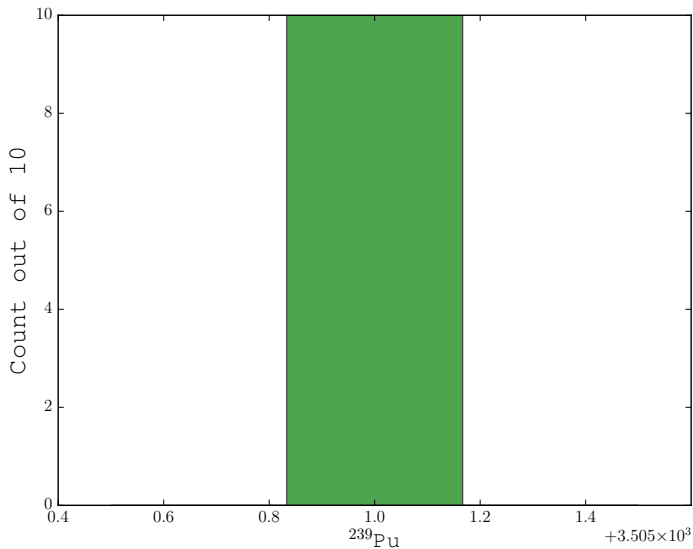


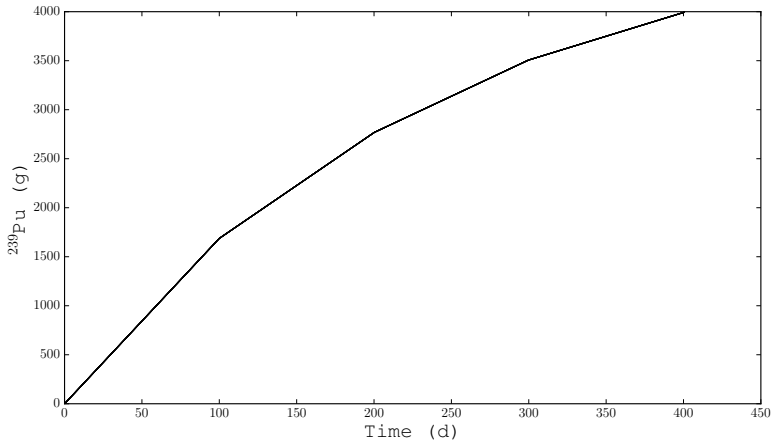


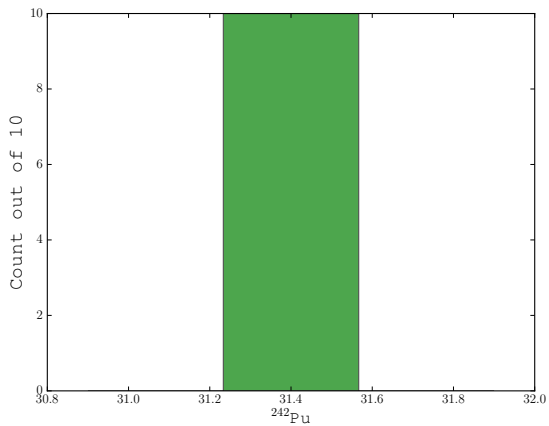
Objectives

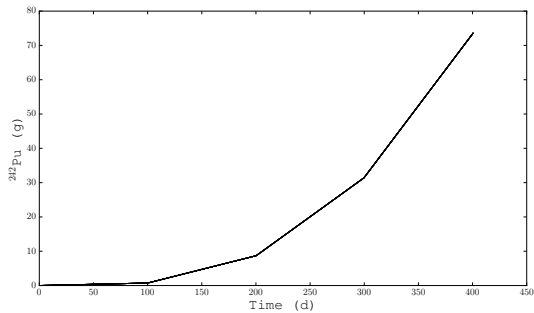
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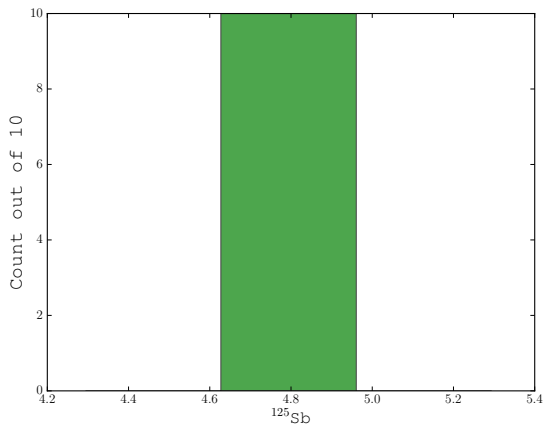
Results

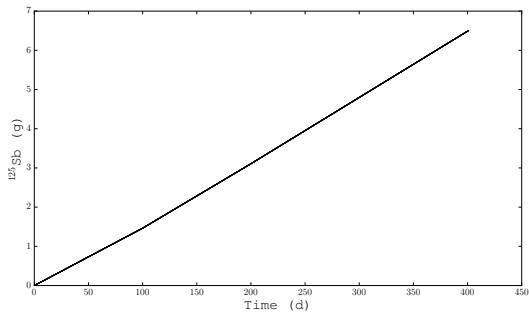


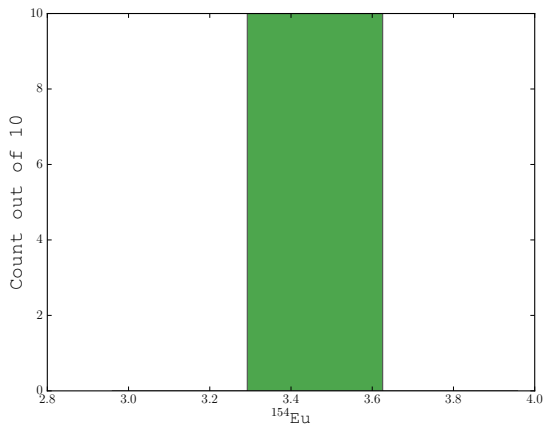


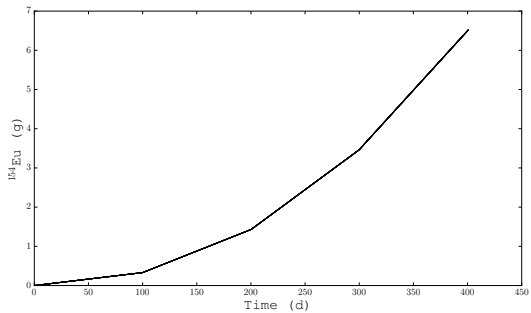


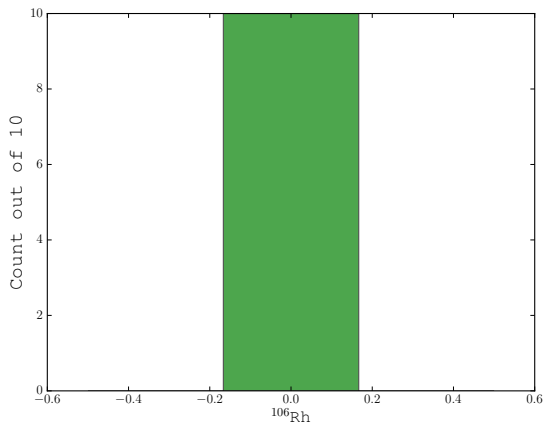


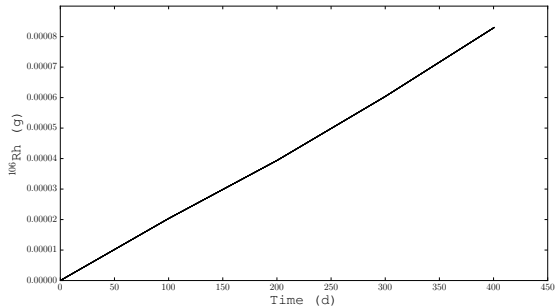


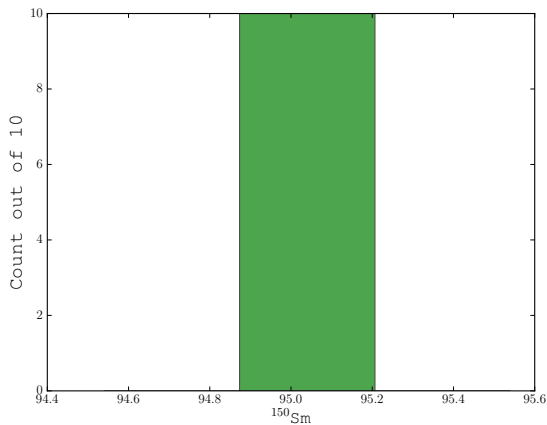


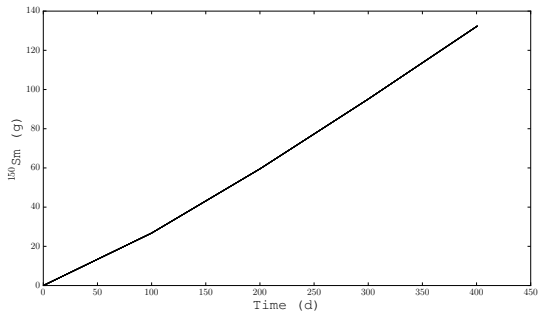


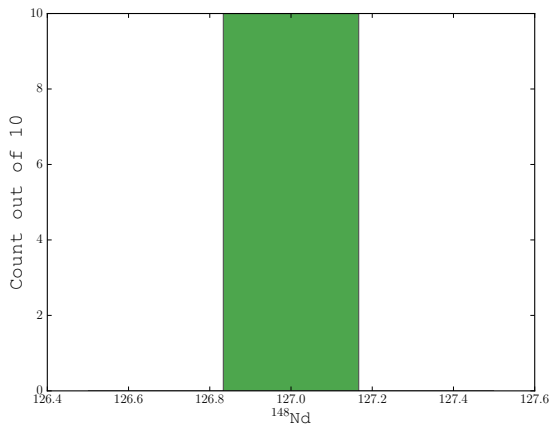


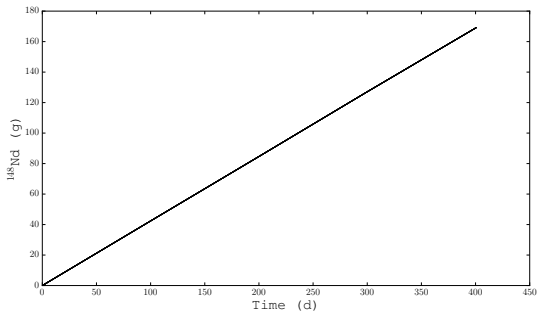


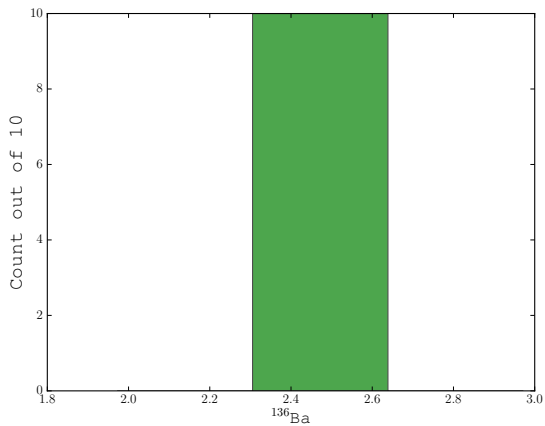


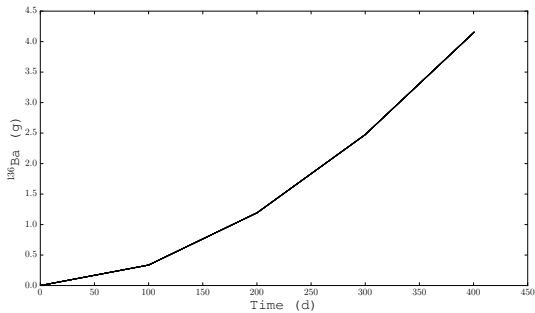


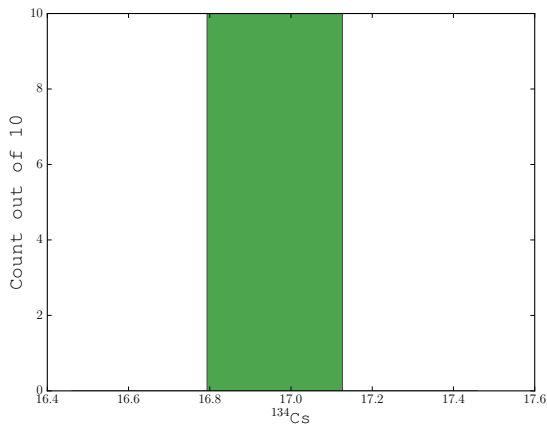


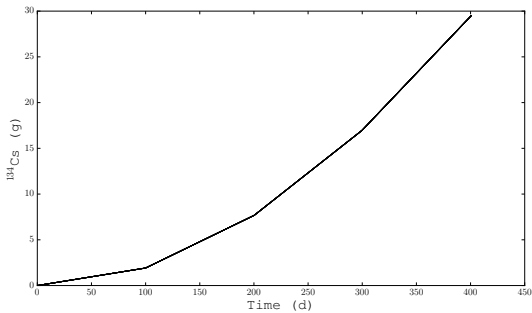












Conclusions

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

