NUEN 647 Final Project

Uncertainty quantification of depletion calculations for specific isotopes using ORIGEN.

I Introduction

Determing composition of irradiated fuel is of importance for a myriad of reasons. Whether for flux calculations, reprocessing, or irradiation history verification, calculating fuel composition requires a Bateman solver, and a means for building a sparse matrix.

Applications using these compositions rarely report the uncertainty associated with results, even when inputs, such as flux shape, fission yield, cross sections, and half-lives have varying degrees of uncertainty. Further sources of error in this calculation are due to the multi-group approximation, and single point approximation, but will not be explored here.

Several isotope concentrations, of interest to the writer, were calculated as a function of burnup with the depletion code ORIGEN2 for a PWR system with 3 Wt% enriched uranium. ORIGEN2 solves the bateman equations with the matrix expoential method and requires a library with decay and cross section information. Cross sections and fission product yields are reduced to single group through flux averaging before execution of the code, with the assumption that the flux has the same shape as a typical PWR.

The uncertainty of concentrations were determined by varying the cross section, fission yeild, and half-life information that was fed into ORIGEN2. The uncertainties on cross sections were determined by calculating the range of the single group cross section, taking the mid point as a mean, the range as a standard deviation, and assuming a Gaussian distribution. A similar calculation was done for the fisison yields, and half-life distributions were taken at face value as normally distributed.

II Objectives

- ☑ Build ORIGEN2 model for thermal system which calculates concentrations of isotopes shown in Table 1.

Listing 1: PWR Input Deck

```
-1
-1
-1
  RDA  Irradiation of 1 MT of PWR fuel
  RDA  Fuel enrichment is 3.0 w/o U-235
  RDA
  LIB  0  1 2 3  601 602 603  9  50 0 1 38
  PHO     101 102 103  10
  INP  1   1  -1  -1   1   1
  BUP
  IRP 100.0 37.5 1 2 4 2 BURNUP=3,750 MWD/MT
  IRP 200.0 37.5 2 2 4 0 BURNUP=7,500 MWD/MT
  IRP 300.0 37.5 2 2 4 0 BURNUP=11,250 MWD/MT
  IRP 400.0 37.5 2 2 4 0 BURNUP=15,000 MWD/MT
  DEC 500.0      2 3 4 0 DECAY FOR 100.0 DAYS
```

```
  DEC 4150.0     3 4 4 0 DECAY FOR 10 YEARS
  DEC 73500.0    4 5 4 0 DECAY FOR 200.0 YEARS
  BUP
  OPTL 24*8
  OPTA 4*8 5 19*8
  OPTF 4*8 5 19*8
  OUT     5   1  -1   0
  END
2 922340 270. 922350 30000. 922380 969730. 0 0.0
0
```

Model irradiates 1 metric ton of US PWR fuel for a single cycle (15,000 MWd/Mt). The calculations use a constant power assumption of 37.5 W/g. The model does not include the oxygen because we are not interested in the activation of oxygen. Cross section modifcation throughout the calculation use the changing flux associated with a US PWR.

Initial verification of the model analyzed the end concentration of ^{137}Cs and calculated the burn-up from that value. This calculation does not have an exact value for the yield of ^{137}Cs and is used qualitatively as a sanity check.

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

- [x] Determine how to vary cross section and or flux spectrum inputs for calculation ORIGEN2 reads in cross section information through a file named “TAPE9.inp”. Cross sections are calculated with This file contains information about single group cross
- [ ] Determine how to vary fission yields for calculation
- [ ] Determine how to vary half-life information for calculation
- [ ] Create a sampling space for all possible variations of calculations
- [ ] Determine importance of various uncertain parameters by running the code a number of times randomly sampling the sample space (still not 100% sure how to do this - not even 50% sure how to do this)

Table 1: Isotope solve list.

^{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

III Quantities of Interest and Uncertain Parameters

Quantities of interest are shown in Table 1 above. Uncertain parameters are listed below:

- Fission yield
- Cross sections
- Half-lives

IV Prediction

The first major prediction for this project is that half-lives will not have a large impact on results because they are relatively well known. Secondly, ^{125}Sb is notorious for being difficult to calculate, I would would predict that there would be large uncertainties due to uncertainties in the cross section data.