INL/CON-23-70855-Revision-0

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May 2023

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Prepared for the
U.S. Department of Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517

Cross-Section Comparison for Pu-238 Production in the Advanced Test Reactor at Idaho National Laboratory

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Qualification of Advanced Test Reactor (ATR) positions for Pu-238 production has been ongoing at Idaho National Laboratory (INL). The ATR qualifications have stretched over multiple years during which new techniques have been developed and made available for ATR experiment neutronic analysis. As part of the transition to newer codes, new cross-section libraries have been evaluated for use in the Pu-238 production experiment analysis. A comparative study was done using the MCNP ORIGEN Activation Analysis (MOAA) tool between ENDF/B-VII.0 and ENDF/B-VIII.0 cross sections to capture the impact of the change in cross-sections on the analysis needed to qualify Pu-238 production targets. All comparisons were done assuming the ATR GEN-I targets were located in the south flux trap of the ATR. Finally, an overview of how this qualification and potential irradiation fits into Pu-238 is discussed.

I. INTRODUCTION

Qualification of multiple Advanced Test Reactor (ATR) positions for Pu-238 production has been ongoing at Idaho National Laboratory (INL) as part of the campaign to restart domestic production of plutonium-238 used in radioisotope power systems (RPS) by the National Aeronautical and Space Administration (NASA) and Department of Energy (DOE) Office of Nuclear Energy (NE), Office of Nuclear Infrastructure Program (NE-3). As part of the qualification process, multiple neutronics analyses have been conducted using different depletion techniques, many of which were developed by INL staff and have been used in many ATR experiment analyses.

The ATR qualifications have stretched over multiple years during which new techniques have been developed and made available for ATR experiment neutronic analysis. As part of the transition to newer codes new cross-sections have been evaluated for use in the Pu-238 production experiment analysis. The purpose of this paper is to document the comparative study between ENDF/B-VII.0 cross sections and ENDF/B-VIII.0 cross sections and the appropriate application for Pu-238 production neutronic analysis in the ATR.

II. Pu-238 PRODUCTION TARGET

The Pu-238 production targets used in the ATR were designed by Oak Ridge National Laboratory (ORNL) and are referred to as ATR-GEN1 targets. Each Pu-238 production target consists of a stack of cylindrical pellets, composed of 20-volume% neptunium oxide (NpO_2), 70-volume% aluminum, and 10-volume% void. Two targets are stacked end-to-end and placed into a basket in order to increase the number of NpO_2-Al pellets irradiated per cycle and to utilize the full length of the ATR, see Fig. 1 and Fig. 2.

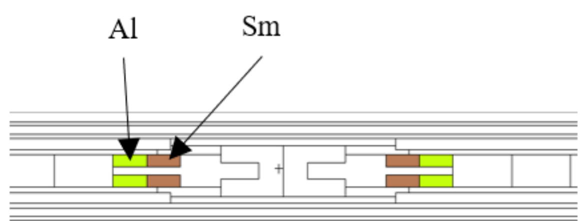

Fig. 1. MCNP axial view of Pu-Production targets.

Fig. 2. MCNP cross section of the ATR.

III. ANALYSIS METHODS

The following codes have been used to qualify the Northeast Flux Trap (NEFT), South Flux Trap (SFT), and I positions in the ATR for Pu-238 production: MCNP [1] [2], ORIGEN2.2 [3] [7], and SCALE6.2 [10]/ORIGENS.

The codes were selected based on what was available when each position was being qualified.

III.A. MOPY

INL staff developed a python-based code coupling MCNP and ORIGEN2, called MOPY [8] (MCNP to ORIGEN2 in Python). MOPY was written using the python scripting language and was developed to manage input file generation, execute MCNP5, extract and manipulate the MCNP output, transfer the data into the ORIGEN2 input file, and execute ORIGEN2. MOPY has been the primary tool for ATR experiment neutronic analysis for many years.

To complete the Pu-238 production target analysis for the NEFT qualification, MOPY was executed for nine timesteps to capture 65 days of irradiation. Each timestep varied from three to ten days in length but all assumed a constant lobe power of 20 MW. Each qualified ATR position was analyzed at a different lobe power, specific to the location. For the Pu-238 production target analysis in the NEFT, approximately 70 nuclides were tracked in MOPY.

III.B. MOAA

The newly developed MCNP ORIGEN Activation Analysis (MOAA) is being used for Pu-238 production neutronic analysis starting in FY23. MOAA is an automation tool that passes data between MCNP and the SCALE modules COUPLE, ORIGEN-S, and OPUS for depletion and activation. MOAA also automates the calculation of the following: mechanistic source term (reported in grams and curies); burnup (reported in %FIMA or MWd/MTU); decay heat (reported in watts); gamma heating (reported in W/cc); neutron heating (reported in W/cc); and the neutron flux for the MCNP cells of interest. The coupling of the two codes is performed using python. The python tool generates the required tallies to track the cells of interest and inserts them into the MCNP model. Once the MCNP model is performed, the tally results are then extracted and fed into the ORIGEN modules. The MCNP to ORIGEN method is repeated for the specified number of timesteps.

IV. Pu-238 PRODUCTION CROSS-SECTIONS

IV.A. ENDF/B-VII.0

To perform the neutronic analysis using MOPY, the ENDF/B-VII.0 [4] cross section library in MCNP was used along with the neptunium-236m cross section library obtained from TENDL-2017 [5]. The standard ATR cross section library was used for ORIGEN2 along with MCNP-calculated replacement cross sections. While multiple nuclides were tracked in MOPY, the tracking of Np-236m (See Fig. 3) was important for tracking production of the impurity Pu-236 and enabling Pu-236 minimization due to significant gamma emitters in the Pu-236 decay chain. To properly track the amount of Np-236m produced from the (n,2n*) reaction, where the * indicates an excited or metastable state, MOPY must be properly set to handle the (n,2n*) reaction. MOPY has three different treatment settings (default, zero, and ratio) for calculating the cross section that leaves a product nucleus in a metastable state, and the ratio setting was deemed most fitting for the PFS target analysis. In the ratio setting, MOPY calculates the ratio of the (n,2n) reaction cross section to the (n,2n*) cross section in the standard cross section library and then applies that ratio to the MCNP-calculated (n,2n) total cross section to the calculate the new (n,2n) and (n,2n*) replacement cross sections used by ORIGEN2.

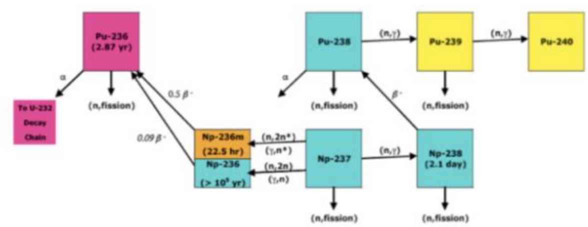

Fig. 3. Nuclear Reactions of Interest for Neptunium Pellet Material.

IV.B. ENDF/B-VIII.0

The ENDF/B-VIII.0 [9] cross section library was released in 2018. The latest release includes many updates to the nuclear data. MOAA was specifically designed to use the ENDF/B-VIII.0 cross section library due to ENDF/B-VIII.0 not containing any elemental cross-section data. Using the ENDF/B-VIII.0 library eliminated the need for the TENDL-2017 library to track the production of Np-236m for the Pu-238 production analysis. ENDF/B-VIII.0 is the preferred cross-section library for all future neutronic analysis in the ATR.

V. CALCULATIONS

To evaluate the impact of changing cross-sections, multiple calculations were performed using both cross-section libraries. The calculations were completed using the MOAA tool. Specific items of interest were the neutron and photon heating rates, average fission density, average Pu-238 assay, average Np conversion, average Pu-236 (ppm), and the Pu-238 yield (grams). All SFT analyses assumed a south lobe power of 25.6 MW.

V.A. HEAT GENERATION RATE CALCULATION

The heat generation rate values were calculated using the MCNP tally type 6 results, the heating normalization factor (HNF) [6], and the ATR core power. Prompt neutron and gamma heating rates (PHR) were calculated using equation (1). The linear heat generation rates were calculated by multiplying the PHR by the MCNP calculated volume and then dividing that product by the segment (in cm).

$$\text{PHR}=(\text{f6})(\text{HNF})(\text{Core Power})\ \frac{W}{g} \qquad (1)$$

V.B. FISSION DENSITY CALCULATION

The fission density was calculated using the output files produced from MOAA. Fission density is a cumulative measure of fissions that have occurred per unit volume in fissionable material and is directly related to burnup. Because each fission typically produces fission fragments that have atomic numbers, Z, less than 90, it can be assumed that every fission removes a heavy metal atom (Z≥90) from the fissionable material. Thus, the fission density, FD, is calculated from the difference between the initial density of heavy metal atoms, $\rho_{initial}$, and the current density of heavy metal atoms, $\rho_{current}$.

VI. RESULTS

VI.A. HEAT GENERATION RATES IN THE SFT

To compare the impacts of changing cross-sections in the qualification of the Pu-238 production targets, multiple analyses of the targets in the SFT were closely compared. The heat generation rates (HGR) for the ATR-Gen1 experiment were calculated using a 3 radial, 7 axial-region fuel model of the ATR. The peak HGR in the neptunium pellet material for each cross-section library is reported in Table 1. Fig. 4 shows the heating profile of the Pu-238 production targets for each cross-section library. The peak HGR for the ENDF/B-VIII.0 cross-section library was 513.12 W/g and the peak HGR for the ENDF/B-VII.0 cross-section library was 486.43 W/g. The ENDF/B-VIII.0 cross-section library provided a more conservative value for the heat generation rates than the ENDF/B-VII.0 counterpart.

TABLE 1. Summary of End of Cycle Heat Generation Rates for Pu-238 Production in the SFT.

Cross-Section Library	Max (W/g)	Min (W/g)
ENDF/B-VII.0	486.43	7.36
ENDF/B-VIII.0	513.12	7.52

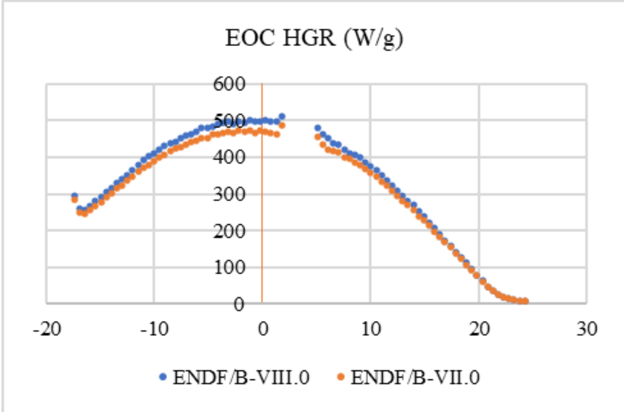

Fig. 4. Maximum heat generation rate profile at the end of 65 days of irradiation using ENDF/B-VII.0 and ENDF/B-VIII.0 cross sections.

VI.B. Pu-238 YIELD IN THE SFT

Table 2 and Table 3 report the average fission density, average Pu-238 assay, average Pu-236 content, and the Pu-238 yield per target for each cross-section library, after 65 days of irradiation, and all were important to capture in the comparison analysis. Of particular interest to the Pu-production design team is the Pu-238 yield for each qualified position in ATR. The estimated yield for each target in the SFT is reported in Fig. 5.

TABLE 2. Estimated Peak Pu-238 Yield in the SFT using ENDF/B-VII.0 cross-sections after 65 days of irradiation.

Target	Average Fission Density (fissions/cc)	Average Pu-238 Assay	Average Pu-236 Content (ppm)	Pu-238 Yield (g)*
Upper Tube 1	1.28E+20	86.0%	3.30	3.86
Lower Tube 1	2.32E+20	80.7%	3.33	5.10
Upper Tube 2	1.25E+20	86.0%	3.16	3.82
Lower Tube 2	2.27E+20	80.8%	3.22	5.06
Upper Tube 3	1.25E+20	85.9%	2.88	3.78
Lower Tube 3	2.27E+20	80.6%	2.94	5.01
Upper Tube 4	1.27E+20	85.7%	2.64	3.77
Lower Tube 4	2.31E+20	80.3%	2.76	4.99
Upper Tube 5	1.27E+20	85.8%	2.86	3.81

Target	Average Fission Density (fissions/cc)	Average Pu-238 Assay	Average Pu-236 Content (ppm)	Pu-238 Yield (g)*
Lower Tube 5	2.32E+20	80.4%	2.95	5.03
Upper Tube 6	1.28E+20	85.9%	3.19	3.85
Lower Tube 6	2.32E+20	80.6%	3.22	5.08
Upper Tube 7	1.10E+20	86.6%	3.12	3.71
Lower Tube 7	2.00E+20	81.7%	3.23	4.91
			Total (g):	61.78
Max	2.32E+20	86.6%	3.33	5.10
Min	1.10E+20	80.3%	2.64	3.71
Average	1.75E+20	83.4%	3.06	4.41

* actual production values may vary

TABLE 3. Estimated Peak Pu-238 Yield in the SFT using ENDF/B-VIII.0 cross-sections after 65 days of irradiation.

Target	Average Fission Density (fissions/cc)	Average Pu-238 Assay	Average Pu-236 Content (ppm)	Pu-238 Yield (g)
Upper Tube 1	1.24E+20	86.1%	3.43	3.83
Lower Tube 1	2.27E+20	80.8%	3.46	5.07
Upper Tube 2	1.22E+20	86.2%	3.27	3.79
Lower Tube 2	2.22E+20	80.9%	3.35	5.03
Upper Tube 3	1.21E+20	86.0%	3.02	3.75
Lower Tube 3	2.22E+20	80.7%	3.08	4.98
Upper Tube 4	1.23E+20	85.9%	2.75	3.74
Lower Tube 4	2.26E+20	80.4%	2.86	4.96
Upper Tube 5	1.24E+20	85.9%	2.96	3.77
Lower Tube 5	2.27E+20	80.5%	3.05	5.01
Upper Tube 6	1.24E+20	86.1%	3.28	3.82
Lower Tube 6	2.27E+20	80.7%	3.33	5.06
Upper Tube 7	1.07E+20	86.8%	3.26	3.68
Lower Tube 7	1.95E+20	81.8%	3.37	4.88
			Total (g):	61.36
Max	2.27E+20	86.8%	3.46	5.07
Min	1.07E+20	80.4%	2.75	3.68
Average	1.71E+20	83.5%	3.18	4.38

* actual production values may vary

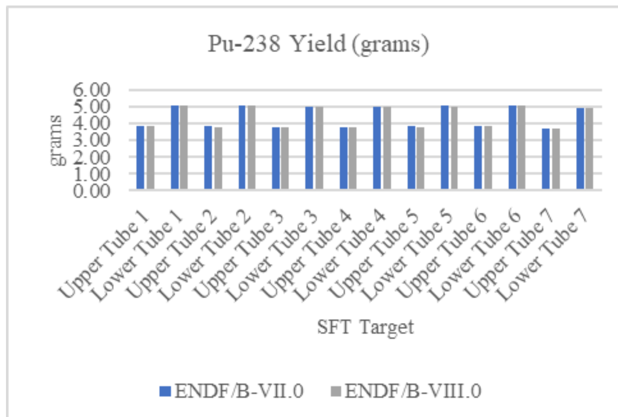

Fig. 5. Estimated Pu-238 yield (grams) at the end of 65 days of irradiation in the SFT using ENDF/B-VII.0 and ENDF/B-VIII.0 cross sections.

VII. CONCLUSIONS

Pu-238 production at Idaho National Laboratory will be completed using ORNL manufactured targets, which are referred to as ATR Generation I Targets. To support irradiation of the ATR GEN-1 targets in multiple ATR positions, multiple analyses were completed using the python-based codes, MOPY and MOAA. MOPY has been the only tool available for ATR neutronic analysis for many years and was written using the python scripting language and developed to manage input file generation, execute MCNP5, extract and manipulate the MCNP output, transfer the data into the ORIGEN2 input file, and execute ORIGEN2. MOPY was specifically designed to work with the ENDF/B-VII.0 cross-sections.

MCNP ORIGEN Activation Analysis (MOAA) is a new python-based tool that was developed by INL staff to replace MOPY. MOAA is an automation tool that passes data between MCNP and the SCALE modules COUPLE, ORIGEN-S, and OPUS for depletion and activation. MOAA is able to utilize older cross-section libraries but was designed specifically to interface with the newest ENDF-B-VIII.0 cross-sections.

A comparative study between ENDF/B-VII.0 and ENDF/B-VIII.0 cross sections to capture the impact on the analysis needed to qualify Pu-238 production targets was performed using the MOAA tool. Specifically, the heat generation rates, average fission density, average Pu-238 assay, average Pu-236 content, and the Pu-238 yield were closely investigated. All comparisons were done assuming the ATR GEN-I targets were located in the SFT of the ATR. The initial differences are acceptable and work continues on the application of the ENDF/B-VIII.0 into the remaining safety analysis.

Final analysis is pending but it is estimated that irradiating 14 ATR GEN-1 targets in the ATR SFT for 65 days of irradiation at a peak power of 25.6 MW will produce a maximum amount 61.4g of Pu-238 with an average assay of 83.5%, which exceeds the minimum 82.5% assay typically used in NASA missions. The continued qualification and production of Pu-238 in the ATR helps INL and DOE meet Pu-238 production goals.

ACKNOWLEDGMENTS

This work was funded by NASA Interagency Agreement # NNH19OB05A and DOE contract DE-AC05-00OR22725 and DE-AC07-05ID14517.

This work also leveraged the High-Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.

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