GENERATING CROSS SECTIONS FOR ORION FUEL CYCLE MODELS

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ABSTRACT

ORION is a fuel cycle modeling tool developed at the UK National Nuclear Laboratory that can be used model once-through, limited recycle, and continuous recycle fuel cycle options. When modeling fuel cycle options with ORION, the fuel within the reactor can either use predefined charge and discharge recipes of spent fuel isotopes or one-group cross sections. Recipes work well for once-through fuel cycle models and steady-state scenarios, whereas cross sections improve accuracy for the more complex scenarios involving isotopic changes that occur during fuel cycle transitions and on the approach to equilibrium. This paper describes the importance of using cross sections based on fuel cycle scenarios, explains the method developed for generating ORION-formatted cross sections with SCALE, and demonstrates the impact of using cross sections versus recipes on fuel cycle analyses.

Key Words: **ORION, Fuel Cycle, Cross Sections, Recipes, US Spent Fuel Inventory**

1. INTRODUCTION

ORION, a nuclear fuel cycle simulator developed at the UK National Nuclear Laboratory (NNL), is designed to simulate the operations of general nuclear fuel cycles, including once-through, limited recycle, and continuous recycle fuel cycle options [1][2]. ORION can simulate the full range of nuclear-related facilities (interim and long-term storage locations, fabrication and enrichment plants, reprocessing facilities, and reactors). It can track over 2,500 nuclides and can model decay and in-reactor irradiation. Based on ORION's ability to track the full isotopic mass flow between fuel cycle facilities (with or without decay), it is possible to model all of the

important nuclide production and destruction routes, which is essential when calculating accurate spent fuel compositions and associated metrics (e.g., decay heat and radioactivity). When modeling a possible transition from one fuel cycle to another, it is important to model the production and destruction routes because during dynamic transition they can vary significantly from their associated steady-state conditions. This paper describes the importance of using cross sections based on fuel cycle scenarios, explains the method for generating ORION-formatted cross sections using SCALE, demonstrates the impact of using these cross sections for fuel cycle transition analysis, and summarizes the results and future work planned for developing cross sections for use in ORION.

2. IMPORTANCE OF CROSS SECTIONS IN TRANSITION ANALYSIS

In ORION, production and destruction routes within a reactor are modeled by using recipes or cross-section libraries. Recipes, which are used by most fuel cycle modeling tools, are tabulated sets of feed and discharge compositions for a given fuel irradiation. They provide the "transfer coefficients" that fuel cycle simulators need to convert mass flow compositions for the feed fuel of a reactor into the mass flow compositions of used nuclear fuel discharged from the reactor. Recipes are calculated ahead of time using neutronics depletion analysis tools and then are input directly into the fuel cycle model. Although this approach is suitable for modeling fuel cycles with a fixed input and output composition (e.g., once-through low-enriched uranium fuel cycles and simple single recycle scenarios) or fuel cycles already at equilibrium when compositions do not very significantly, it is difficult to accurately model more complex scenarios involving isotopic changes that occur during transition and on the approach to equilibrium. This includes changing from one fuel type to another or from one fuel cycle approach to another, such as transitioning from the current U.S. LWR fleet to a fleet of molten salt U/Pu reactors.

Using problem-specific cross-section libraries generated by neutronics depletion tools is the second method for modeling production and destruction routes within ORION. Unlike the recipes method, the output stream in the reactor model is dynamic and changes on the basis of input stream composition. Another advantage of using cross-section libraries within ORION is that it has a built-in cross-section interpolation routine that generates reactor-, cycle-, and scenario-specific production and destruction routes during the fuel cycle calculation. This provides a means to capture the effects of changes in the neutron flux spectrum and magnitude have on isotopic concentrations and cross sections during transition.

3. METHOD FOR GENERATING CROSS SECTIONS WITHIN ORION

Oak Ridge National Laboratory (ORNL) has collaborated with NNL to produce additional burnup-dependent cross-section libraries that are specific to the fuel cycles being evaluated in the DOE Fuel Cycle Options (FCO) campaign [3]. The cross sections for thermal spectrum systems were generated with the SCALE suite of codes [4]. A schematic of the process and interfaces, both within SCALE and the interface between SCALE and ORION, is shown in Figure 2.

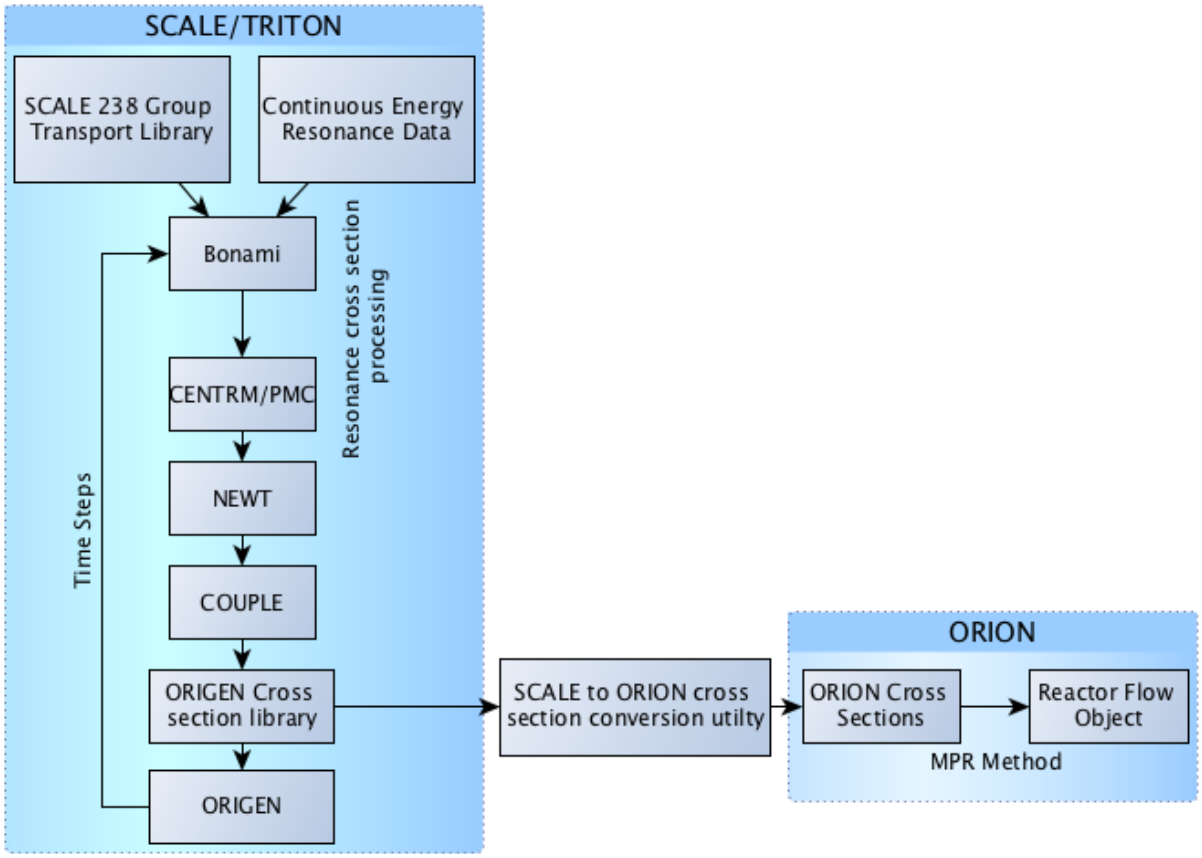

Figure 1. Schematic of link between SCALE and ORION.

Bonami and CENTRM/PMC are resonance cross-section processing codes used to generate a problem specific self-shielded corrected multigroup cross-section libraries set used by NEWT. NEWT is a two-dimensional multigroup discrete-ordinates transport code used to calculate the reactor's energy-dependent flux. The energy-dependent flux is then used with COUPLE (the library management code for ORIGEN) to collapse the 238-group cross-section library into a one-group cross-section library. The one-group cross-section library is then fed into ORIGEN (an irradiation and decay code) to calculate the depleted material compositions that are then fed back into Bonami and CENTRM/PMC. A more detailed description of the codes within SCALE used for creating reactor-, burnup-, and enrichment-specific microscopic cross sections can be found in the SCALE manual [4]. The four steps discussed above are repeated for the number of irradiation decay steps specified. This process can then be repeated for multiple perturbations to the reactor model, including changes to various feed fuel parameters (e.g., ^{235}U enrichment, total Pu fraction, total fissile fraction, and Pu isotopic vector), all of which can be interpolated within ORION.

However, the cross sections generated with SCALE are in a format different from that required by ORION. Therefore, processing tools were developed to format the one-group SCALE cross sections into ORION cross-section libraries. These steps allowed for development of reactor-specific, burnup-dependent cross sections for multiple perturbations to the reactor models.

Currently, the method described above has been used to generate enrichment- and burnup-dependent ORION cross-section libraries for a pressurized water reactor (PWR) and a boiling water reactor (BWR), as well as a burnup-dependent cross-section library for a thorium-fueled molten salt reactor (MSR). The cross section generation method described above will have limitations on generating cross sections for fast spectrum system. For fast spectrum systems, a similar method is being developed where a different reactor physics code such as MCNP [6], a continuous energy Monte Carlo neutronics code, will replace NEWT in the method described above. In addition, work is ongoing to develop cross sections for other fuel cycle scenarios.

4. RESULTS

The importance of using cross sections for more complex scenarios can be seen in Figure 3. Recipes and one-group cross sections were generated for a W17x17 [5] assembly with an initial enrichment of 4.21 wt% U-235 and a discharge burnup of 50 gigawatt-days/metric tons of heavy metal (GWd/MTHM). The enrichment and burnup values were based on parameters used to generate recipes for the LWR fuel for the Nuclear Fuel Cycle Evaluation and Screening Study [3]. The cross sections were generated for a range of enrichments and burnups. These recipes and cross sections were then used to model a different reactor configuration, which consisted of the W17x17 with an initial enrichment of 2.9 wt % U-235 and a discharge burnup of 30 GWd/MTHM. The enrichment and burnup values were based on the average enrichment of U.S. PWR spent fuel between 1968-1983 [7]). The differences between the results from all three methods were then compared against a TRTION/SCALE neutronic calculation. Results from specifying the production and destruction routes using recipes, one-group cross sections, and interpolated cross sections are shown in Figure 3.

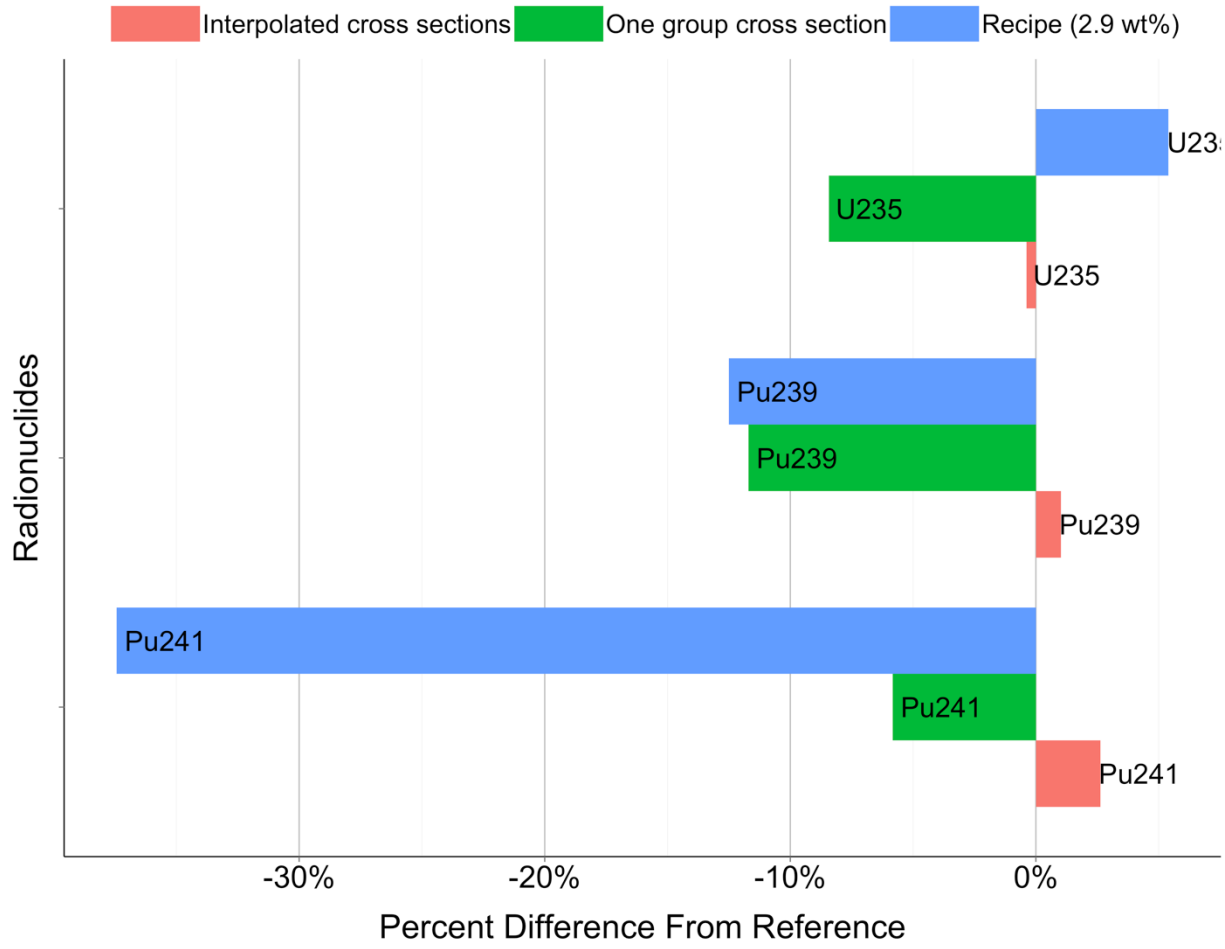

Figure 2. The percent differences between recipes, a single set of cross sections, and cross sections with interpolation compared against a reference TRITON calculation.

As expected, the results from the burnup- and enrichment-dependent cross sections most closely approximated the reference neutronics results calculated with TRITON, whereas the recipe produced the least accurate results. In this simple steady-state example, it would be simple enough to generate recipes for the different LWR configurations. However, the use of recipes for modeling fuel cycle scenario transitions would not be as accurate as using cross sections, especially when the spent fuel composition changes over time and these changes are not known beforehand.

To demonstrate further the improved accuracy of interpolated cross sections as compared to recipes, a comparison was performed on the current US spent fuel inventory. This was performed by comparing results calculated from using cross sections and recipes against assembly-by-assembly calculated radionuclide values found within the Used Nuclear Fuel—Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS) Unified Database [8].

UNF-ST&DARDS is a comprehensive, integrated data and analysis tool developed to support US Department of Energy (DOE) spent nuclear fuel (SNF) management and fuel cycle activities. UNF-ST&DARDS provides a unified domestic SNF system database, referred to as the Unified Database (UDB). The UDB is integrated with nuclear analysis capabilities to characterize input to the SNF management system; provide a credible, controlled data source for key information; assess issues and uncertainties related to the extended storage and transportability of loaded canisters; support research and development prioritization; and preserve SNF-related information. Data within the UDB that is pertinent to the comparison include:

- assembly by assembly information, including
  - burnup, enrichment
  - metric tons of initial heavy metal (MTHM)
  - cycle history
  - assembly types for each assembly
- properties for different assembly types, including
  - fuel pin characteristics
  - assembly array characteristics
  - burnable poison rod characteristics
  - guide tube characteristics
  - instrument tube characteristics

In addition to data found within the UDB, UNF-ST&DARDS has built-in tools that allow for automating the generation of ORIGEN/SCALE cross-section libraries for each unique assembly type, depletion of each individual assembly, and decay of each assembly to a specific date. Because of the detailed calculations along with the extensive collection of data within the UDB, it was assumed that the radionuclide results stored within the UDB would be a good standard for comparing the differences between using cross sections and recipes in modeling fuel cycles.

For the comparison, the total uranium, average burnup, and average enrichment for the US spent fuel data within the UDB was aggregated into 5-year increments as seen in Table 1 and Table 2 for BWR and PWR respectively. As seen in these tables, average burnup ranges from around 11 GWd/MTHM to 47 GWd/MTHM, and average enrichment ranges from around 2.1 wt % U-235 to 4.3 wt % U-235, once again demonstrating the wide variation in the burnup and enrichment of SNF over time.

The radionuclide results used to compare the differences between cross sections and recipes came directly out of the UDB for an evaluation date at 2025. As mentioned above, the values within the UDB include radionuclides calculated for every spent fuel assembly in the United States up to 2013 and take into account the enrichment, burnup, cycle time, and assembly type for each individual assembly.

Table 1. Discharged US BWR assemblies binned by five-year increments up to 2013

Bin range (year)	Total uranium (MTHM)	Average burnup (MWd/MTHM)	Average enrichment (wt % U-235)
1968–1969	10.5	15,850	2.06
1970–1974	551.1	10,850	2.23
1975–1979	1,690.1	18,320	2.15
1980–1984	2,415.8	24,790	2.53
1985–1989	2,823.1	22,890	2.38
1990–1994	3,275.2	29,260	2.75
1995–1999	3,746.9	35,110	3.17
2000–2004	3,536.3	40,000	3.56
2005–2009	3,430.5	43,300	3.87
2010–2013	2,651.5	44,560	4.01

Table 2. Discharged US PWR assemblies binned by five-year increments up to 2013

Bin range (year)	Total uranium (MTHM)	Average burnup (MWd/MTHM)	Average enrichment (wt % U-235)
1970–1974	458.1	20,520	3.14
1975–1979	2,602.0	24,710	2.71
1980–1984	3,632.9	29,870	2.93
1985–1989	5,455.8	31,990	3.08
1990–1994	7,135.5	37,300	3.49
1995–1999	7,458.1	41,640	3.84
2000–2004	7,277.0	45,930	4.17
2005–2009	7,559.3	46,810	4.28
2010–2013	5,125.1	45,880	4.30

The cross sections used for the comparison were calculated with ORIGEN/SCALE using a SCALE-generated Westinghouse 17x17 low patristic (LOPAR) [5] fuel assembly design for the PWR fuel assemblies and a General Electric 10x10 fuel assembly GE-14 design for the BWR assemblies [5]. The cross sections were used to interpolate on enrichment and burnup, and the results were scaled by the total mass. All of the results were decayed to the year 2025; for example, the fuel assemblies discharged in 1969 decayed for 56 years, whereas the fuel assemblies discharged in 2013 decayed for only 12 years.

The recipes used for the comparison were obtained from the Evaluation Group 1 fuel cycle scenario associated with the recent US DOE Nuclear Fuel Cycle Evaluation and Screening Study [3]. The radionuclides obtained from the recipes were decayed to the year 2025 based on the binning structure. Then these decayed radionuclides were scaled for each bin range (years) according to the total mass specified in Table 2. Finally, all of the results from each bin range (years) were summed together to obtain the calculated radionuclide concentration at 2025 for all of the spent fuel assemblies discharged before 2013.

The results obtained from the UDB, interpolated cross sections, and recipes along with the differences between the UDB and cross sections and the differences between the UDB and recipes can be seen in Table 3. The radionuclides chosen for the comparison were the important nuclides contributing to decay heat for typical LWR fuel for cooling times from about 1 to 1,000 years [9] along with U-235 and U-238. These radionuclides were used because they are important for analyzing the tail end of the fuel cycle for such things as storage, recycling/reprocessing, and permanent disposal.

In Table 3 the more significant differences between using recipes and cross sections are highlighted purple (U-238, U-235, Pu-239, and Cs-137) and the radionuclides where the cross sections comparison result has a larger relative error then recipes are highlighted in yellow (Ru-106, Pm-147, Pu-241). The percent differences between the UDB and cross sections and between the UDB and the recipes are visually displayed in Figure 3.

Table 3. Nuclide masses evaluated at the year 2025 for a subset of radionuclides within SNF from the UDB compared with ORION-calculated masses using cross-sections and recipes

Radionuclides	UDB (reference) [MTHM]	Cross sections [MTHM]	Recipe [MTHM]	Difference between UDB and cross sections (MTHM)	Difference between UDB and the recipe (MTHM)
Sr-90	2.17E+01	2.31E+01	2.91E+01	-1.37E+00	-7.43E+00
Y-90	5.50E-03	5.85E-03	7.57E-03	-3.48E-04	-2.07E-03
Ru-106	2.25E-04	5.67E-04	5.13E-04	**-3.42E-04**	-2.88E-04
Sb-125	6.64E-03	8.24E-03	1.20E-02	-1.60E-03	-5.37E-03
Cs-134	2.61E-02	4.32E-02	4.58E-02	-1.71E-02	-1.97E-02
Cs-137	5.30E+01	5.60E+01	6.99E+01	-2.95E+00	**-1.69E+01**
Pm-147	7.69E-02	1.22E-01	8.25E-02	**-4.51E-02**	-5.62E-03
Eu154	3.85E-01	4.45E-01	7.16E-01	-6.03E-02	-3.32E-01
U-235	7.48E+02	7.15E+02	5.21E+02	3.38E+01	**2.27E+02**
U-238	6.63E+04	6.56E+04	6.48E+04	6.80E+02	**1.44E+03**
Pu-238	1.58E+01	1.41E+01	1.87E+01	1.66E+00	-2.95E+00
Pu-239	5.34E+02	5.38E+02	4.34E+02	-4.66E+00	**9.95E+01**
Pu-240	1.83E+02	1.88E+02	2.09E+02	-5.05E+00	-2.63E+01
Pu-241	3.60E+01	4.02E+01	3.86E+01	**-4.20E+00**	-2.58E+00
Am-241	8.61E+01	8.41E+01	8.91E+01	1.96E+00	-2.97E+00
Cm-242	1.36E-04	1.35E-04	7.77E-05	9.95E-07	5.83E-05
Cm-244	2.08E+00	1.91E+00	2.29E+00	1.65E-01	-2.13E-01

Of the three radionuclides that had larger differences between the UDB and the interpolated cross sections compared to the differences between the UDB and the recipe, the most significant one for fuel cycle modeling is Pu-241 because it is fissile. However, for fuel cycle analysis this is expected to have a minimal effect on the overall results. This is because the differences are only 0.5% of the total calculated Pu within the fuel and only 0.3% of the calculated fissile material within the fuel.

Of the larger differences between the UDB and the recipe, the most significant differences are U-235 and Pu-239 because they are both fissile. For example, as shown in Table 3 the interpolated cross sections underpredicted the amount of fissile material by 25 MTHM (around 2% of the total fissile material), whereas the recipes underpredicted the amount of fissile material by 300 MTHM (around 25% of the total fissile material). These differences are especially significant for fuel cycle analyses that often heavily rely on the amount of fissile material waiting to be recycled.

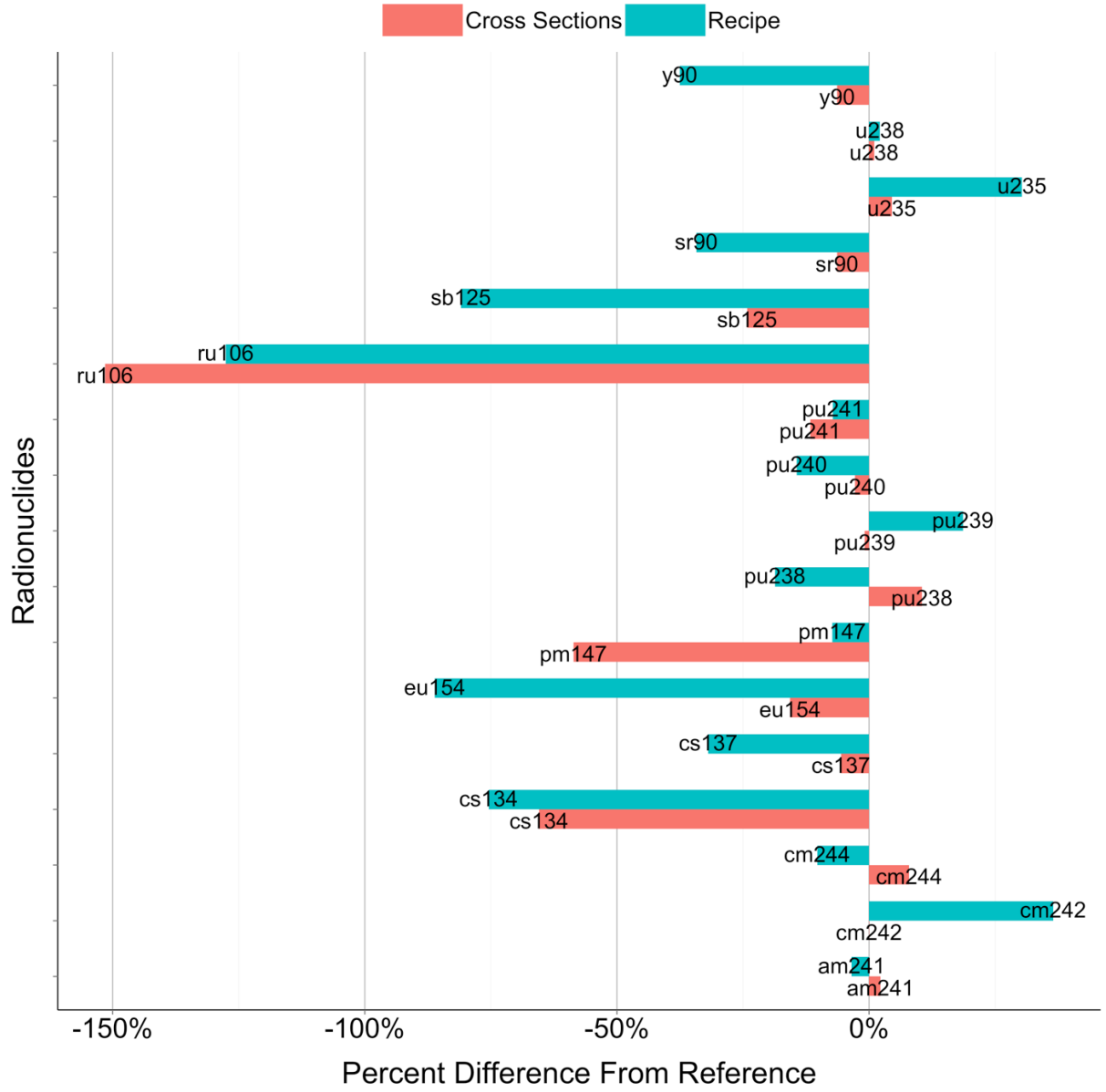

Figure 3. Comparison between the percent differences from UNF-ST&ARDS and the results obtained from using cross sections and recipes evaluated at the year 2025.

It should be noted that if the recipes were generated from all 20 state points within Table 1 and Table 2, then the results from the recipes should be much closer to the UNF-ST&DARDS database results. However, this would increase the time required to generate the recipes, and if the binning structure changed, then new recipes would need to be regenerated, increasing the time even more. With interpolated cross sections, once the cross sections have been generated, the data's binning structure can be changed without adding significant computational time for fuel cycle calculations.

5. CONCLUSION

ORION can model fuel cycles using either recipes or cross sections. As demonstrated in this paper, recipes work well for static systems such as once-through fuel cycle models and steady-state scenarios, whereas cross sections have the ability to capture changes in more dynamic systems such as complex scenarios involving the multi-reuse and isotopic changes that occur during transition and on the approach to equilibrium. SCALE is now being used to develop cross-section libraries for ORION, including multi-region cross sections. A comparison between interpolated cross sections and recipes showed that cross sections provide for the most part a more accurate result when the spent fuel parameters vary greatly from the initial assumptions used to generate the recipes.

Future work with ORION and cross sections includes developing more ORION-usable cross-section sets for different reactors and configurations. In addition, research is being performed to determine if the new ORIGEN API available in SCALE 6.2 could be used for directly modeling the irradiation and decay calculations within ORION, potentially enabling the development of additional interpolations schemes for fuel cycle transition analysis.

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