INL/EXT-12-26804

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The INL is a U.S. Department of Energy National Laboratory
operated by Battelle Energy Alliance

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

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August 2, 2012
INL/EXT-12-26804

Prepared in partial fulfillment of the requirement of the Department of Energy's Science Undergraduate Laboratory Internship under the direction of Samuel E. Bays in the Reactor Physics Analysis and Design division at Idaho National Laboratory.

This paper was prepared for the U.S. Department of Energy Office of Nuclear Energy, Science, and Technology under DOE Idaho Operations Office Contract DE-AC07-05ID14517.

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Abstract

When modeling the behavior of a nuclear reactor over time, it is important to understand how the isotopes in the reactor will change, or transmute, over that time. This is especially important in the reactor fuel itself. Many nuclear physics modeling codes model how particles interact in the system, but do not model this over time. Thus, another code is used in conjunction with the nuclear physics code to accomplish this. In our code, Monte Carlo N-Particle (MCNP) codes and the Multi Reactor Transmutation Analysis Utility (MRTAU) were chosen as the codes to use. In this way, MCNP would produce the reaction rates in the different isotopes present and MRTAU would use cross sections generated from these reaction rates to determine how the mass of each isotope is lost or gained. Between these two codes, the information must be altered and edited for use. For this, a Python 2.7 script was developed to aid the user in getting the information in the correct forms. This newly developed methodology was called the Coupled Reactor Depletion Instrument with Automated Controls (CRDIAC).

As is the case in any newly developed methodology for modeling of physical phenomena, CRDIAC needed to be verified against similar methodology and validated against data taken from an experiment, in our case AFIP-3. AFIP-3 was a reduced enrichment plate type fuel tested in the ATR. We verified our methodology against the MCNP Coupled with ORIGEN2 (MCWO) method and validated our work against the Post Irradiation Examination (PIE) data. When compared to MCWO, the difference in concentration of U-235 throughout Cycle 144A was about 1%. When compared to the PIE data, the average bias for end of life U-235 concentration was about 4%. These results from CRDIAC therefore agree with the MCWO and PIE data, validating and verifying CRDIAC. CRDIAC provides an alternative to using ORIGEN-based methodology, which is useful because CRDIAC's depletion code, MRTAU, uses every available isotope in its depletion, unlike ORIGEN, which only depletes the isotopes specified by the user. This means that depletions done by MRTAU more accurately reflect reality. MRTAU also allows the user to build new isotope data sets, which means any isotope with nuclear data could be depleted, something that would help predict the outcomes of nuclear reaction testing in materials other than fuel, like beryllium or gold.

List of Acronyms

AFIP: Advanced Test Reactor Full Size Plate in Center Flux Trap Position

ATR: Advanced Test Reactor

CRDIAC: Coupled Reactor Depletion Instrument with Automated Control

GUI: General User Interface

HPC: High Performance Computing

INL: Idaho National Laboratory

IDE: Interactive Development Environment

LANL: Los Alamos National Laboratory

MCNP: Monte Carlo N-Particle

MCWO: MCNP Coupled with ORIGEN2

MRTAU: Multi-Reactor Transmutation Analysis Utility

PIE: Post Irradiation Examination

1. Introduction

When material is subjected to a flux of neutrons, the isotopes that make up that material become depleted. This means that those isotopes undergo nuclear reactions with the neutrons and transmute into different isotopes. Thus, there is a deficiency of the isotopes that underwent the nuclear reactions. When designing experiments and fuel to be put into nuclear reactors, it is important to know how these materials will be depleted over time. In order to do this, depletion methodologies are developed. These methodologies normally involve the use of two types of codes in order to simulate the depletion of the material in question.

One of these codes is the nuclear physics code that simulates how the particles interact with the material. These interactions are captured by outputting the reaction rate for each isotope that is being depleted. The other type of code handles how the mass of the isotopes changes due to the reported isotope reaction rate, which is translated into a nuclear reaction cross section. The newly computed composition of the material is reflected in the nuclear physics code, and the cycle is repeated until the appropriate amount of time has elapsed in this burn cycle.

Current depletion simulations are mainly carried out using ORIGEN2 based methodology coupled to MCNP. The goal of this research was to develop an alternative to these methodologies using a depletion code other than ORIGEN2. An additional goal was to broaden the capability of the isotopes that could be depleted. The end product was the Coupled Reactor Instrument with Automated Controls (CRDIAC). This paper will focus on the components that make up CRDIAC, the code's validity, the results from running the code, what those results mean, and what the future of CRDIAC is.

2. The Components of CRDIAC

In CRDIAC, the chosen nuclear physics code was Monte Carlo N-Particle (MCNP). Specifically, MCNP5 version 1.60 was used. CRDIAC's depletion code was the Multi-Reactor Transmutation Analysis Utility (MRTAU). The link between the two codes was developed in Python 2.7 to transform and transfer the data from one code to the other between each run. This Python script is ran as a combination of a number of different modules. Figure 1, below, shows how CRDIAC runs the codes together.

This methodology and others like it that use this back and forth, iterative way of modeling the way the material depletes have an inherent flaw that will keep them from obtaining the exact results from reality. This is due to the fact that each amount of time that the current configuration is burned, or burn step, must have some finite amount of time in order to function. This means that the cross sections of the initial concentrations are used even though, in reality, the cross sections would change every time an atom is lost or gained. This means that the simulation will never be perfectly reflective of reality, so this must be kept in mind whenever a simulation's results are viewed.

Figure 1: CRDIAC Flow of Information Chart

a. MCNP

The nuclear physics code in CRDIAC, MCNP5 version 1.60, was developed by Los Alamos National Laboratory (LANL) and is based on reactor transport theory. It uses Monte Carlo methods to solve the transport equation, which means that many particles are introduced into the system and the path of each particle is tracked and recorded, forming a picture of what would happen in the real life system (1). MCNP includes many options for tracking many different types of reactions with materials using different tallies.

In CRDIAC, volume based neutron flux tallies (f4 tallies) for each depleted, or burned, cell are used to generate the normalized neutron flux. Flux multiplier cards for each isotope in each cell are used to determine the reaction rate for each isotope, which can be transformed into a cross section to be used in the depletion code. Additionally, the criticality eigenvalue calculation (kcode) is also used for the power scaling when determining the true neutron flux, along with a neutron heating tally (f7 tally) for the different lobes of the reactor.

b. MRTAU

MRTAU, the depletion code in CRDIAC, was initially developed by Dr. Sam Bays as part of his PhD work and was further developed at Idaho National Laboratory (INL). MRTAU currently has 29 actinides and 180 fission products that are tracked (2). When used in CRDIAC, almost all of the cross sections for these isotopes are replaced by the ones calculated from MCNP. In this way, the calculation more accurately reflects reality than calculations that do not replace in such a high level of detail. An additional feature of MRTAU is that the user, with proper nuclear data, can add other isotopes to MRTAU for depletion if they are not already present. Such could be the

case with beryllium, which is described in Appendix A. The output from MRTAU is a table of the new concentrations of the isotopes in cm^2/b.

c. Python

In order to speed up the process of coupling MCNP to MRTAU, a series of Python modules were developed to carry out the transformation and translation of the resulting data. Python was chosen because, as a scripting language, it was relatively easy to pick up. Python is also easy to edit the text of the various input and output files with and is also a very portable code, so it can easily be switched to different operating systems. Currently, the process is not fully automated and requires some user attention between running MCNP and MRTAU. Right now, the user would be required to:

1. Run the properly formatted MCNP input file/ put the burn information into info.py
2. Run python on the MCNP output file
3. Transfer the MRTAU input files to the appropriate directories
4. Run MRTAU for each cell
5. Update the MCNP input file with the MRTAU output masses
6. Start the cycle again

d. Operating Environment

The operating system which was used in the development of CRDIAC was Ubuntu Linux on a Dell Optiplex 755 with an Intel Core2 Duo E6550 processor at 2.33GHz and 8 GB of RAM. On this machine, the Python modules were developed using the open source interactive development environment (IDE) IDLE. The MCNP and MRTAU runs were conducted on the INL High Performance Computing (HPC) server Icestorm, which is an SGI Altix ICE 8200 distributed memory cluster that consists of 256 compute blades with two quad core 2.66 GHz Intel Xeon processors per blade (3).

3. Validation and Verification

After CRDIAC's components were in place, it was important to verify that the code returned similar values when compared to another code that did the same task and to validate the code's results against reality in the form of experimental data. The verification was performed against the MCNP Coupled with ORIGEN2 (MCWO) methodology currently used at INL to simulate the depletion of the fuel in the Advanced Test Reactor (ATR). The validation was performed against the data take from the Post Irradiation Examination (PIE) of the same experiment. In this case, the experiment chosen to do the verification and validation was the Advanced Test Reactor Full Size Plate in Center Flux Trap Position (AFIP) experiment, AFIP-3. AFIP-3 was a reduced enrichment plate type fuel tested in the ATR, located in the center flux trap, shown below in Figure 2. It was run for ATR Cycles 143B and 144A, where it shared the AFIP assembly with AFIP-1 in the former and a dummy plate in the latter (4).

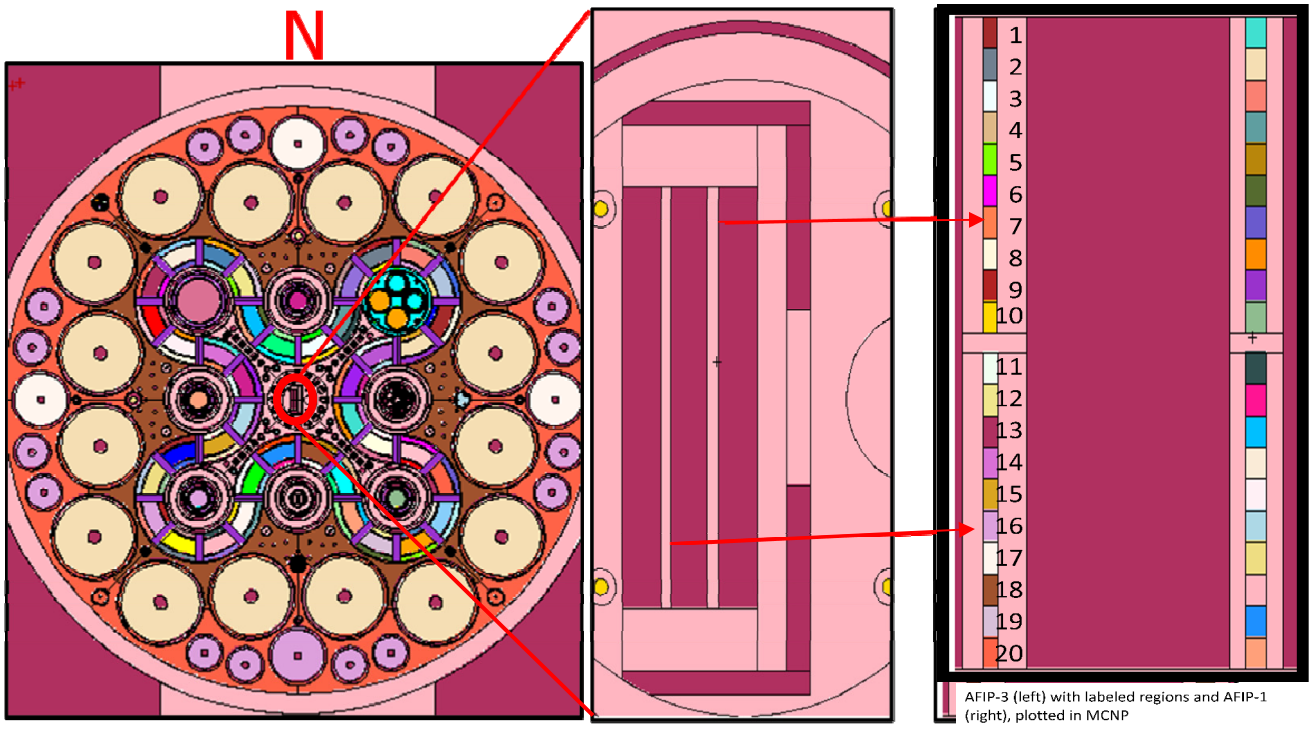

Figure 2: From left to right, top view of ATR, top view of the AFIP-1(left) and -3 (right) experiments, side view of the AFIP-1 and -3 experiments.

By performing these comparisons, CRDIAC could be considered a working code if its results did fit the results obtained by other means. By verifying CRDIAC, it would be clear that it worked in a similar way as a currently used methodology. By validating CRDIAC, it would be clear that it reflects what actually happens in the nuclear system.

4. Results

After running CRDIAC for the same experiment and circumstances present in the real life experiment and the as-run simulation performed with MCWO, the results from CRDIAC were compared to the other two means. Figure 3, below, shows the comparison of the MCWO and CRDIAC U-235 concentrations present in the first region during Cycle 144A, illustrating the verification results. Table 1, below, shows the difference in the atomic percents of U-235, U-238, and the Cs-134/Cs-137 ratio at the end of life calculated in CRDIAC and from the PIE chemical analysis, illustrating the validation results. Figure 4, below, illustrates the ability for CRDIAC to show how the U-235 concentration and the Cs-134/Cs-137 ratio look at the end of life for the fuel. From the figure, it is evident that the cells that experience a higher burnup (toward the center) had lower concentrations of U-235 and higher Cs-134/Cs-137 ratios, which is what one would suspect based on nuclear physics. Figures 5 and 6 show the gamma scan of the AFIP-3 plates compared to the CRDIAC concentrations for Cs-137 and Nb-95, respectively.

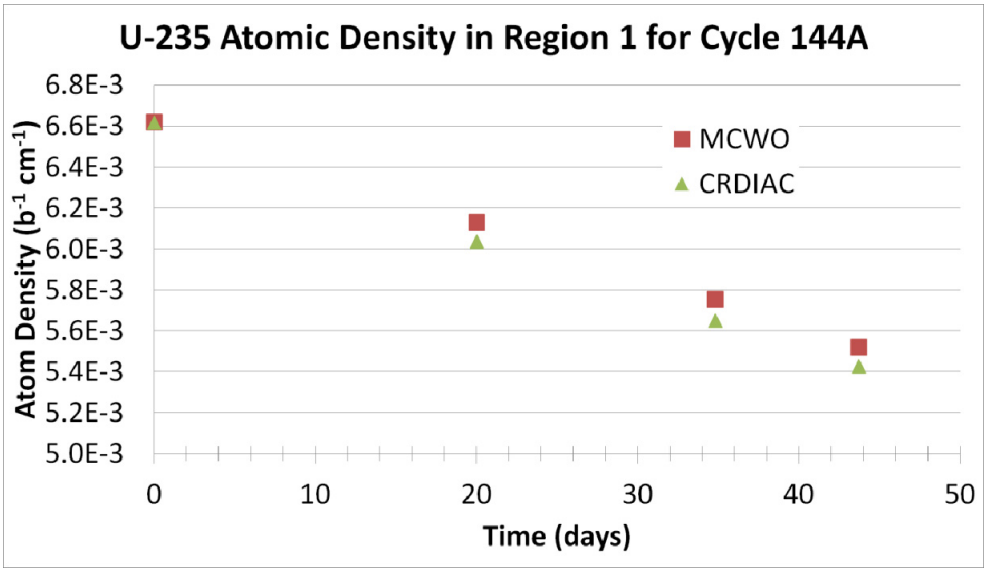

Figure 3: Verification of CRDIAC compared to MCWO for AFIP-3 (4)

Table 1: Validation of CRDIAC against PIE data for AFIP-3 (5)

Computed/Experimental Isotopic Ratio				
Region 7				
Isotope	**CRDIAC**	**Experiment**	**C/E**	**Bias**
U-235	8.34%	9.23%	0.903	9.693%
U-238	90.00%	88.39%	1.018	-1.817%
Cs134/Cs137	3.84%	3.76%	1.020	-2.034%
Region 3				
Isotope	**CRDIAC**	**Experiment**	**C/E**	**Bias**
U-235	11.18%	11.16%	1.002	-0.203%
U-238	87.07%	86.81%	1.003	-0.294%
Cs134/Cs137	3.01%	3.12%	0.963	3.704%
Region 14				
Isotope	**CRDIAC**	**Experiment**	**C/E**	**Bias**
U-235	7.30%	7.07%	1.032	-3.220%
U-238	90.23%	90.15%	1.001	-0.094%
Cs134/Cs137	4.42%	4.87%	0.906	9.434%
Region 18				
Isotope	**CRDIAC**	**Experiment**	**C/E**	**Bias**
U-235	9.21%	9.50%	0.969	3.053%
U-238	88.66%	88.15%	1.006	-0.579%
Cs134/Cs137	3.80%	4.10%	0.926	7.378%

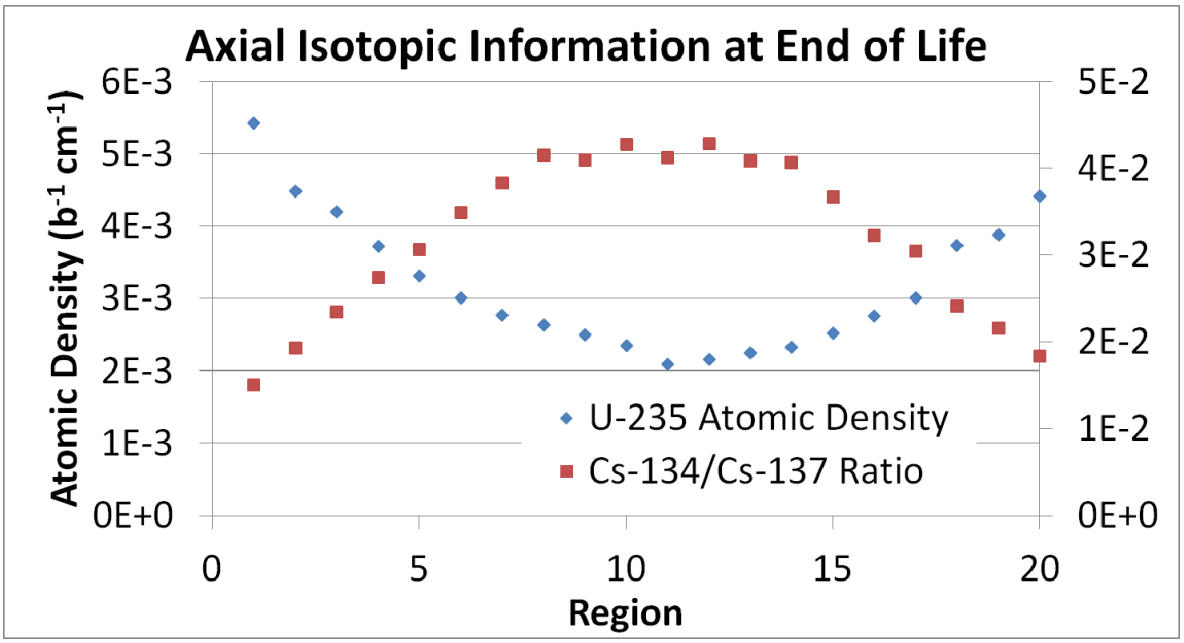

Figure 4: CRDIAC output used to show the axial difference of U-235 and the Cs ratio at end of life for AFIP-3

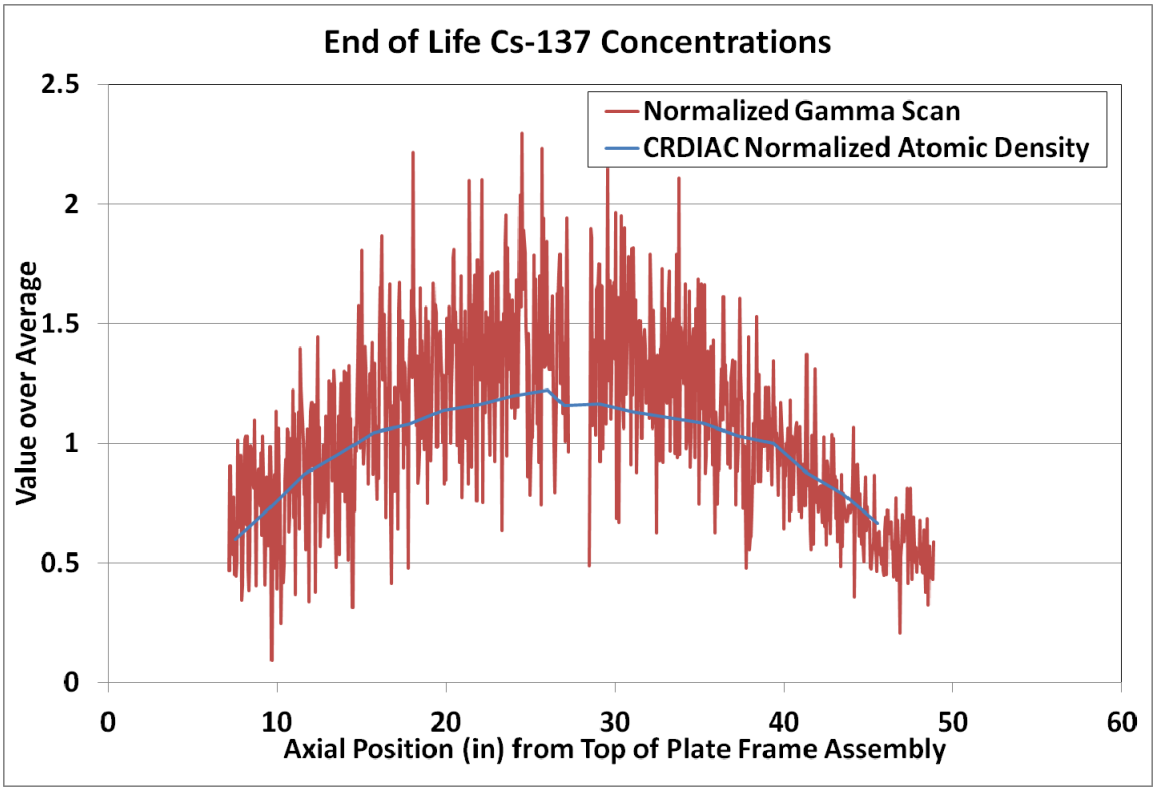

Figure 5: CRDIAC Cs-137 concentrations compared to the PIE gamma scan for AFIP-3(5)

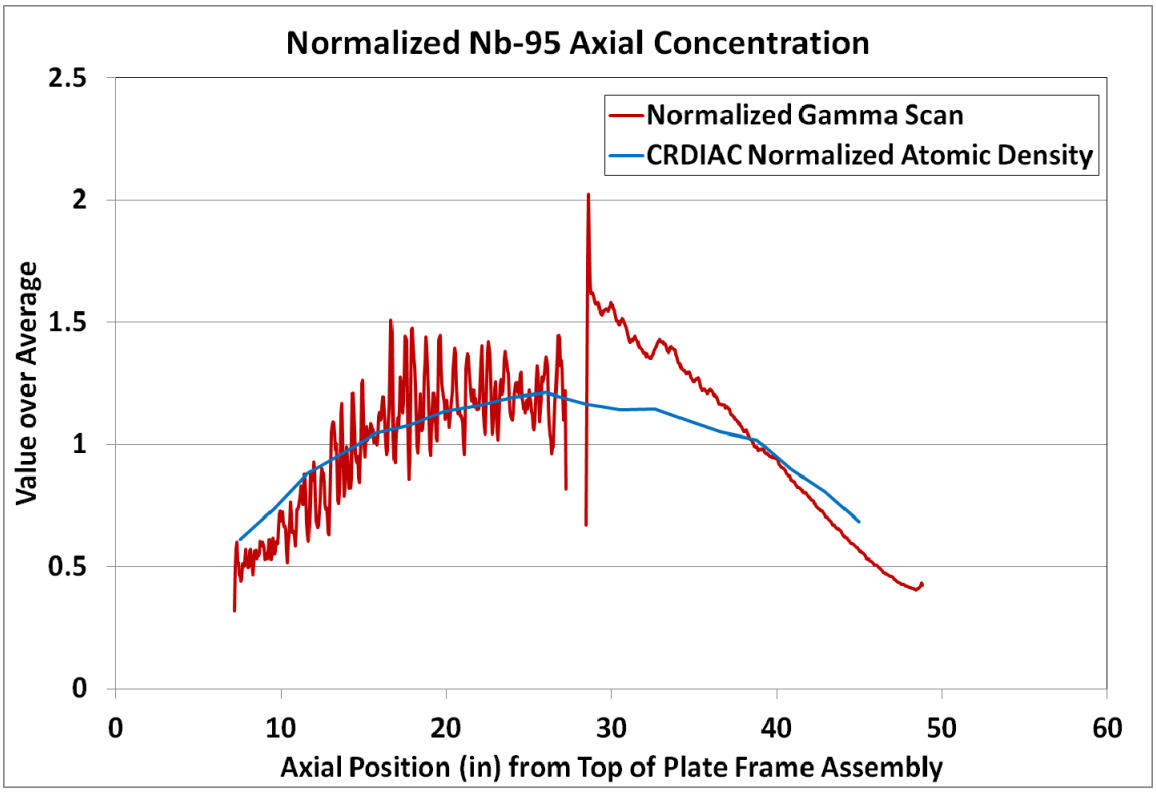

Figure 6: CRDIAC Nb-95 concentrations compared to the PIE gamma scan for AFIP-3(5)

5. Conclusions

After comparing the MCWO and CRDIAC data for U-235 concentration in region 1 throughout Cycle 144A (Figure 3), the standard deviation between the data points at each time in the cycle was about 1.2% on average, so this was concluded to pass the verification step (raw data in Appendix B). The comparison of CRDIAC to the chemical analysis for the different regions (Table 1) for U-235 concentration varied in bias, as the region 3 sample yielded about a .2% bias and the region 7 sample yielded about a 9.7% bias, while the other two regions yielded about 3% biases. Taken together, the average bias was about 4%, so these results are still close enough to validate CRDIAC. The biases may be reduced if the cell volumes were decreased in the MCNP model of the experiment, which would lead to more cells being burned and more MRTAU calculations, producing a finer image of the how the fuel is burned. The above gamma scans and CRDIAC mass data were normalized to produce a comparative representation of the whole plate's isotopic concentration. It is evident by the above graphics that CRDIAC produces results that follow a similar shape as the real life scenario. In conclusion, CRDIAC provides a versatile and user customizable method to deplete fuel or even other materials present in a neutron flux and an alternative to ORIGEN-based methods.

6. Future Work

For the near future, our goal is to get CRDIAC fully automated to the point of having to just press run in the beginning and let CRDIAC do the rest. This would allow the use of CRDIAC in the background so that other work could get done at the same time. A future goal after full

automation would be to have the user interact with a general user interface (GUI) instead of having to mark up their MCNP input file or hardcode into the inof.py module to indicate which cells are burned. This would make using CRDIAC a lot more straight forward and user friendly. A long term goal would be to run MCNP and MRTAU in parallel, cutting down the needed computing time for each burn.

Acknowledgements

I would like to thank all of my mentors for their guidance and assistance during my internship; Sam Bays, Misti Lillo, and Danielle Perez. I would also like to thank Andrea Alfonsi for all of his assistance with MRTAU during my internship. Finally, I would like to thank the Department of Energy for funding my internship and the INL for providing a means to conduct my internship.

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Appendix A: Beryllium Memorandum

This memorandum outlines the needed developments of the Multi-Reactor Transmutation Analysis Utility (MRTAU) in order to implement this code in the depletion of beryllium. The motivation for this comes from the depletion modeling of the Advanced Test Reactor (ATR) at the Idaho National Laboratory (INL), which is largely comprised of beryllium in the form of reflectors to moderate neutrons. The modeling of beryllium is currently not supported by depletion modeling methodologies but is being considered due to the high cross sections of some of its daughter isotopes. Currently, MRTAU is being used by the Coupled Reactor Depletion Instrument with Automated Control (CRDIAC) in conjunction with Monte Carlo N-Particle (MCNP) codes to perform depletions of the given reactor system. In this way, MCNP creates the reaction rates for each isotope that can be depleted in MRTAU and these reaction rates are transformed into cross sections to be used in MRTAU by CRDIAC. CRDIAC also updates the MCNP material compositions after each MRTAU run is complete, allowing for burn cycles to be carried out completely.

The nuclear reaction types of beryllium are summarized in Figure 1 below. They include n,γ; n,α; n,p; and n,2n. The beryllium reaction chains also include β^--decay. All of these reaction and decay types are possibly supported by MRTAU, although some may not be directly supported at the moment.

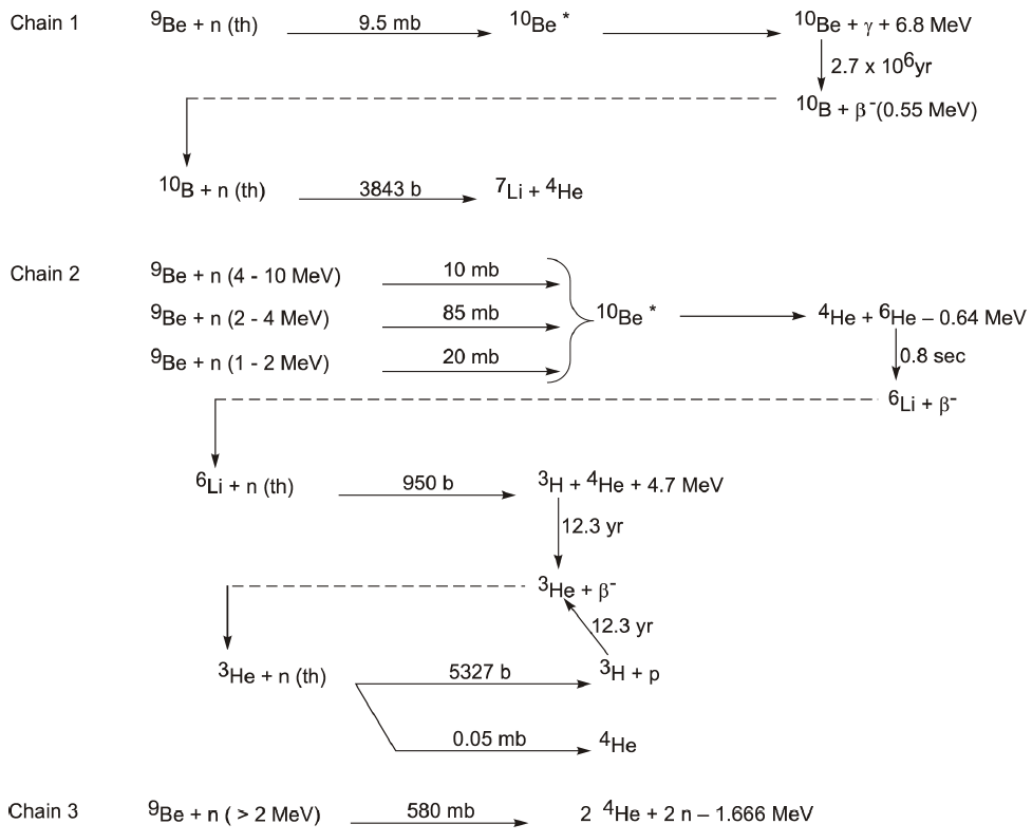

Figure 1: Neutron Beryllium Reaction Chains (1)

Table 1, below, summarizes exactly how the above chains from Figure 1 would be inserted into MRTAU to give MRTAU the ability to deplete beryllium.

Chain	Reaction/Decay	MRTAU Reaction/Decay Type	Comments
1	$^{9}Be + n(th) \rightarrow {}^{10}Be + \gamma$	n,γ	
1	$^{10}Be \rightarrow {}^{10}B + \beta^{-}$	β¯Decay	
1	$^{10}Be + n \rightarrow {}^{7}Li + \alpha$	n,α	
2	$^{9}Be + n \rightarrow {}^{6}He + \alpha$	n,α	^{6}He has no MCNP cross section data
2	$^{6}He \rightarrow {}^{6}Li + \beta^{-}$	β¯Decay	
2	$^{6}Li + n \rightarrow {}^{3}H + \alpha$	n,α	
2	$^{3}He + n \rightarrow ({}^{3}H + p) or\ \alpha$	n,p or n,α	The n,α has no other product
2	$^{3}H \rightarrow {}^{3}He + \beta^{-}$	β¯Decay	Forms a loop with the above reaction
3	$^{9}Be + n \rightarrow 2\alpha + 2n$	n,2n	The 2α comes from the fast decay of Be-8, so it is really an α and a He-4

The isotopes and their reactions and decays in chain 1 are already included in MRTAU, so their nuclear data would just need to be added into the appropriate library data files. Also, the isotopes in chain 1 are available in the nuclear data cross section libraries for MCNP, so their reaction rates can be calculated.

Most of the isotopes and their reactions and decays in chain 2 are supported by MRTAU and would just need to be edited into the library data files. The reaction involving He-3 and a neutron, however, has a probability of being either an n,α or an n,p reaction. In the n,α case, there is no other product, so that would have to be accounted for in MRTAU. He-6, however, does not have any MCNP cross section data associated by it, so this data would need to be attained and put into the MCNP cross section library format. Otherwise, the other isotopes are accounted for in the MCNP cross section libraries.

The two He-4 produced in chain 3 are not directly supported at the moment. A possible solution to this could be to double the branching ration for the production of He-4 from this reaction type, which could be considered n,2n. The 2 He-4 could also be more accurately considered an α and a He-4, because they come from the alpha decay of Be-8. It should also be noted that the decay of Be-8 is almost immediate, 81.9 as (2). Another solution could be to add in this isotope to MRTAU, although nuclear data for Be-8 does not exist in current MCNP5 cross section libraries.

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Appendix B: Raw Data for Comparisons

Comparison of Isotopic Results from MCWO and CRDIAC for U-235 in Cell 8502					
Time(days)	**MCWO**	**CRDIAC**	**Std Dev**	**Raw CRDIAC Data**	**Cell Volume(cm)**
0	6.6180E-03	6.6172E-03	0.01%	4.26E-03	0.6439
20	6.1310E-03	6.0363E-03	1.56%	3.89E-03	
34.8	5.7540E-03	5.6487E-03	1.85%	3.64E-03	
43.7	5.5200E-03	5.4269E-03	1.70%	3.49E-03	

EOL Isotropic Axial Concentrations					Raw Data						
Region	**U-235**	**Cs-137**	**Nb-95**	**z pos**	**U-235**	**Cs-137**	**Nb-95**	**Cs-134**	**134/137**		**vol**
1	5.43E-03	5.82E-01	6.27E-01	7.5	3.49E-03	4.29E-05	2.82E-06	6.47E-07	1.51E-02		6.44E-01
2	4.48E-03	7.06E-01	7.54E-01	9.56	2.89E-03	5.19E-05	3.39E-06	1.01E-06	1.94E-02		
3	4.20E-03	8.48E-01	9.07E-01	11.62	2.71E-03	6.24E-05	4.08E-06	1.47E-06	2.35E-02		
4	3.73E-03	9.29E-01	9.89E-01	13.68	2.40E-03	6.83E-05	4.45E-06	1.88E-06	2.75E-02		
5	3.32E-03	1.01E+00	1.08E+00	15.74	2.14E-03	7.47E-05	4.85E-06	2.29E-06	3.07E-02		
6	3.01E-03	1.05E+00	1.11E+00	17.8	1.94E-03	7.73E-05	5.00E-06	2.70E-06	3.49E-02		
7	2.77E-03	1.11E+00	1.17E+00	19.86	1.78E-03	8.15E-05	5.26E-06	3.13E-06	3.84E-02		
8	2.64E-03	1.13E+00	1.19E+00	21.92	1.70E-03	8.32E-05	5.36E-06	3.45E-06	4.15E-02		
9	2.50E-03	1.16E+00	1.23E+00	23.98	1.61E-03	8.57E-05	5.52E-06	3.51E-06	4.10E-02		
10	2.36E-03	1.19E+00	1.25E+00	26.04	1.52E-03	8.74E-05	5.62E-06	3.74E-06	4.28E-02		
11	2.10E-03	1.19E+00	1.25E+00	27.29	1.51E-03	8.76E-05	5.64E-06	3.62E-06	4.13E-02		7.20E-01
12	2.16E-03	1.20E+00	1.71E-02	29.35	1.55E-03	8.81E-05	7.68E-08	3.77E-06	4.28E-02		
13	2.25E-03	1.16E+00	1.23E+00	31.41	1.62E-03	8.55E-05	5.52E-06	3.49E-06	4.09E-02		
14	2.33E-03	1.14E+00	1.23E+00	33.47	1.68E-03	8.36E-05	5.52E-06	3.40E-06	4.07E-02		
15	2.52E-03	1.11E+00	1.18E+00	35.53	1.81E-03	8.19E-05	5.29E-06	3.01E-06	3.67E-02		
16	2.76E-03	1.06E+00	1.13E+00	37.59	1.99E-03	7.79E-05	5.06E-06	2.51E-06	3.23E-02		
17	3.01E-03	1.03E+00	1.09E+00	39.65	2.16E-03	7.56E-05	4.92E-06	2.31E-06	3.05E-02		
18	3.73E-03	8.99E-01	9.63E-01	41.71	2.69E-03	6.61E-05	4.33E-06	1.60E-06	2.42E-02		
19	3.88E-03	8.11E-01	8.69E-01	43.77	2.80E-03	5.97E-05	3.91E-06	1.29E-06	2.16E-02		
20	4.41E-03	6.83E-01	7.35E-01	45.83	3.18E-03	5.03E-05	3.30E-06	9.26E-07	1.84E-02		
				Averages	2.16E-03	7.36E-05	4.50E-06				