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Modeling Tungsten Boride Neutronics in ORIGEN for Z-Facility

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Abstract

ORIGEN is one of the main transmutation software packages used in nuclear engineering Modeling Tungsten Boride Neutronics in ORIGEN for Z-Facilityproblems. For the case of this study, tungsten borides are studied using a coupled framework between MCNP and the ORIGEN package of scale. The input used four compositions of tungsten boride: WB with natural boron-10 abundance, WB with 80wt% B-10 per isotope of boron, WB4 with natural boron-10 abundance, and WB4 with 80wt% B-10 per isotope of boron. Isotopic inventories were produced for WB which show the time dependent change up to 2 years after a 6-Month irradiation. This will allow for further studies of the materials to assess things material composition changes, dose contribution, and waste management requirements.

Introduction

The Z-Machine at Sandia National Laboratories is a pulsed power facility for fundamental science research. This facility is used for nuclear fusion research which uses many different experimental setups including wire array loads, liners, gas puffs, flyer plates, and short circuits. [1] The facility operates within the nanosecond timescale, offering approximately 1 shot per day for 150 shots per year. Each shot produces load energies of around 3 Megajoules at a peak current of around 26 MA using DT and DD fusion sources. [1] The machine is split into three major material regions: a vacuum chamber, a water section, and an oil section containing Marx Capacitors for power storage. In 2016, a Z-Machine overview presentation reported that the Z-Facility planned for anywhere between 140 and 160 shots with an average of one shot per day except for containment shots (3-6 days per shot). [1] During each shot, material is destroyed calling for a large effort to refurbish the machine for the next shot. While undergoing maintenance, the fluid (water and oil) is drained while components are replaced, and diagnostics are reset. During each shot, very complex radiation fields are produced causing activation of the structural and operational materials. This creates a complicated work environment for technicians, as the drained fluids can no longer moderate radiation, which means that dose rates

will increase to personnel. One final added complexity is the addition of sky shine within the facility. This is the streaming of radiation through unrestricted regions of the problem geometry which then reflect off molecules in the atmosphere. These reflected particles can cause serious issues for activation and personnel dose which must be considered with complex transport modeling and transmutation studies.

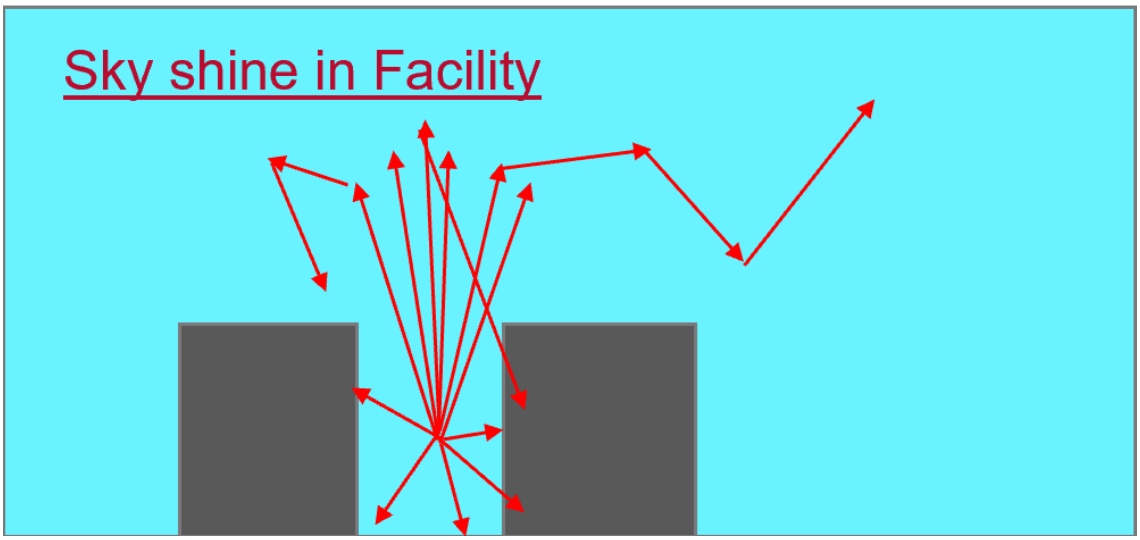

Figure 1: Sky shine in a generic pulsed power facility demonstrating the particle streaming types of concern for transmutation and dose studies.

The main purpose of this project is to find new ways to mitigate radiation hazards to personnel as well as equipment within the complicated environments present. To do this, adequate shielding is required in the facility to minimize dose accumulation in workers, activation of materials, and damage to components of the system. Traditionally, neutron shielding is comprised of light element, hydrogen-based materials or other materials like cement and heavy metals. Examples of the first group include hydrocarbons like high density polyethylene and even water, especially for neutron moderation. It can be advantageous, however, to have a material that is cheaper to make while absorbing neutrons more effectively by using certain isotopes. This is achievable by borating a material that fits the needs of the project at hand. This is because Boron-10, which makes up approximately 18% of natural boron, has an extremely high neutron absorption cross section. Furthermore, the boron can be enriched to higher values of B-10 than is naturally abundant which can increase the effectiveness of the shielding. This is already done in nuclear reactor systems to manufacture nuclear control rods, which act as a neutron poison by absorbing a large part of the neutron population.

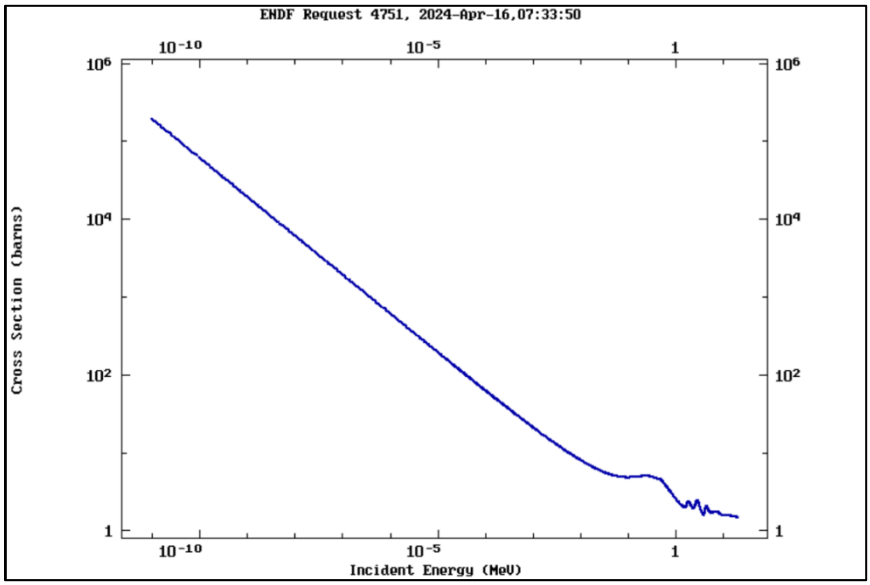

Figure 2: Boron-10 total neutron reaction cross section adapted from ENDF data set on NNDC libraries. [3]

Although not cheap to manufacture, the material in which this research is centered around is the class of tungsten borides. Tungsten is commonly used in these fusion environments for diagnostics and plasma facing materials and can provide attenuation for photons and x-rays. Combined with boron, tungsten could effectively provide adequate biological or equipment shielding for a multispecies radiation field providing that it is not activated or damaged beyond maximum allowable values. The analysis in ORIGEN will provide a starting place to access the activation of the materials as well as a base point to begin research for fundamental material science issues in tungsten borides.

Since the working environments for personnel can become complicated, it is crucial to be able to predict conditions beforehand with computational models. MCNP is the standard tool for modeling radiation transport, however it is limited to linear solutions. Standard assumptions, such as time independence for solutions, constant material compositions, and no inclusion of physical material properties limits the program's ability to model conditions common in nuclear transmutation studies. One work around is to solve an MCNP problem for a set time and use numerical methods to solve the Bateman system. This can work; however, one still needs to update the isotopic inventories which are constantly changing in a true physical system. This is perfect for the application of a transmutation program such as CINDER and ORIGEN. For the study presented, ORIGEN from the SCALE package will be used to investigate the possibilities

of transmutation packages. ORIGEN solves the traditional Bateman system for a user defined set of nuclides given by the equation:

$$\frac{dN_i}{dt} = \sum_{j \neq i}\left(l_{ij}\lambda_j + f_{ij}\sigma_j\Phi\right)N_j(t) - \ (\lambda_i + \sigma_i\Phi)N_i(t) + S_i(t) \qquad [1]$$

In this equation, l_{ij} is the fractional yield of nuclide I from decay of nuclide j, f_{ij} is the fraction yield of nuclide I from neutron induced removal of nuclide j, λ_{ij} is the decay constant of nuclide i, N_i is the number of atoms, Φ is the angle- and energy-integrated time dependent neutron flux , and S_i is the time dependent source term. [2] The solution methodology is split into separate categories: short-lived nuclides and long-lived nuclides. From this, the program generates problem dependent transition matrices and solves the system. This matrix is:

$$a_{ij} = \begin{cases} l_{ij}\lambda_j + f_{ij}\sigma_j\Phi & i \neq j \\ \lambda_i - \sigma_i\phi & otherwise \end{cases} \qquad [2]$$

This stores reactions with flux values of one and then later in the solution replaces this with a solved step-average flux. The removal cross section and reaction yields are then generated for further calculations. The actual solution process is completed via one of two solving methods that are native to ORIGEN: MATREX and CRAM. MATREX is the hybrid matrix exponential/linear chains method which solves the standard ODE of the form:

$$\vec{N}(t) = \exp(\boldsymbol{A}t)\,\vec{N}(0) \qquad [3]$$

Where the exponential term is expanded via Taylor expansion and solved:

$$\exp(\boldsymbol{A}t) = \boldsymbol{I} + \boldsymbol{A}t + \frac{(\boldsymbol{A}t)^2}{2} + \cdots = \sum_{k=0}^{\infty}\frac{(\boldsymbol{A}t)^k}{k!} \qquad [4]$$

The second method is the Chebyshev Rational Approximation Method, CRAM. This method has similar runtimes compared to MATREX and is more accurate as it relies on LU decomposition. It is also more robust for a large range of problems making it a good option for many problem types.

The final consideration is the problem boundaries. For a generic pulsed power machine, the shot schedule and geometry need to be considered. For the case of a proof-of-concept solution in ORIGEN, one must consider a month shot schedule. In ORIGEN, the input file

requires that time points be defined within a matrix with a matching flux value. This means for a matrix of 30 days with 1day increments, there must be 30 corresponding flux values. The second consideration is the input geometric model for radiation transport. One method of achieving this is by running radiation transport computations in MCNP and then using a calculated flux as an input value in the ORIGEN code. ORIGEN requires that each input file requires that a data library be generated in multigroup form up to 200 groups. This means that the MCNP flux would serve as a good baseline for transmutation modeling. Finally, a great method of creating geometric models in MCNP is the use of Atilla4MC by SilverFir Software. This program is very useful for generating unstructured meshes from CAD models and then automatically importing them in to an MCNP input file.

Method

This paper focuses on a generalized Z-Machine pulsed power system with a simple variable shot scheme. In this case, the machine will ideally operate for 5 days per week with a yield of 10^{14} neutrons per shot and a high yield shot of 10^{21} neutrons every 30 days. The ORIGEN code will be used to track the activation of material through neutron capture as well as the decay of radioisotopes between shots. The geometric model in consideration is a simple "3 region" model in which there is a vacuum stack, water section, and oil section all contained by some structural material (in this case SS316).

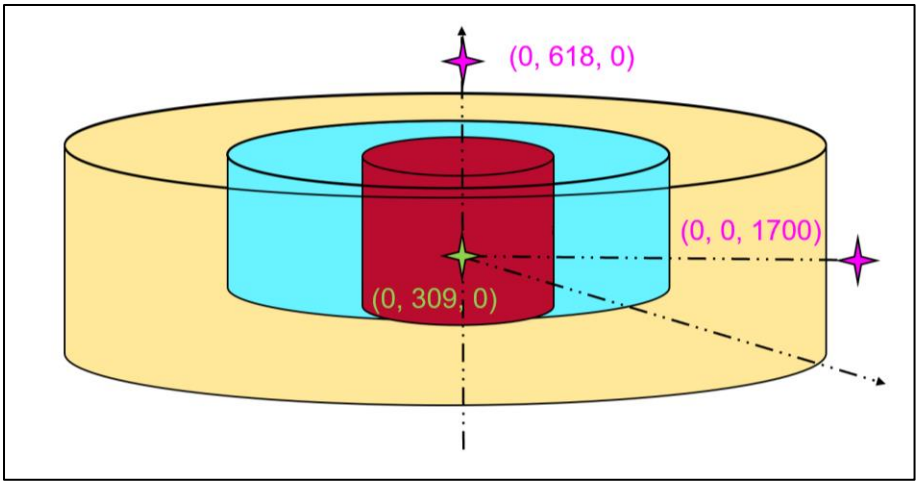

Figure 3: Simple Z-Machine styled model for use in Atilla4MC containing vacuum, water, and oil sections.

In this model, there are three total point detectors which are used to calculate neutron energy distributions at the desired locations. For proof of concept, the reported results will only look at

the values at the topmost location (0, 618,0). This will provide a first estimate for looking at sky shine physics within a facility as well as a good region for sampling a partly thermalized neutron energy spectrum. In future studies, it will be more beneficial to run detector calculations using a realistic detector model in order to produce more accurate results.

The ORIGEN files were separated into 6-month time increments. This allows one to calculate the nuclide inventories up to 6 months of shot data and then load the nuclide inventories into a file for the next 6 months and iterate. ORIGEN also requires that an initial isotopic inventory be stated in some way; in the case of this project, WB is specified as an atom density composition calculated for each WB_x type in a separate data file. It became clear that the typical shot nanosecond timeframe produced inaccurate solutions. It is believed that since the time scales were vastly different between each shot and the total 6-month time frame, that the program would mistake some time points as being the same. For this case, one-second-long shots were used in the simulations which is certainly a point of inaccuracy and will need to be adjusted for future simulations.

Results

Based on the above framework, simulations were run for WB and WB_4 compositions. These were chosen because they represent the low and high bounds for boron concentration. Each value was calculated with boron concentrations at natural B-10 and 80wt% B-10 enrichment.

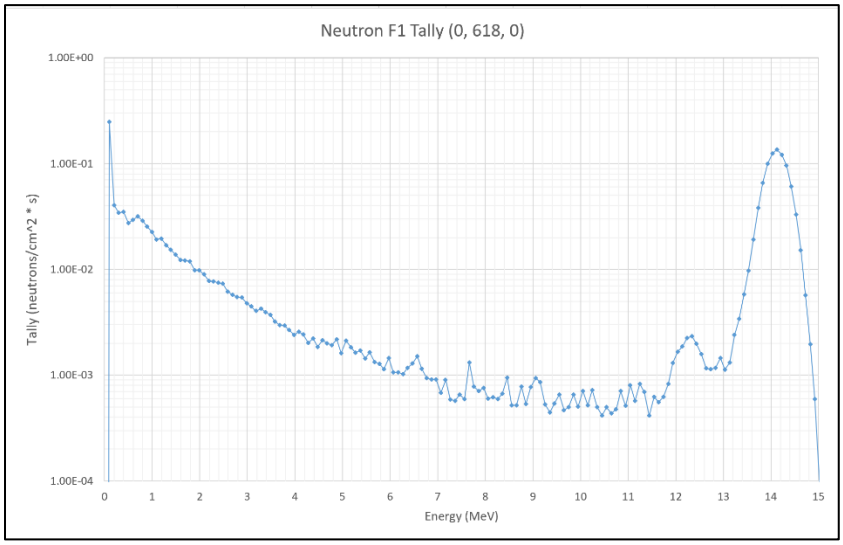

Figure 4: Neutron energy spectrum generated in MCNP for the location (0, 618, 0) within the facility model used as an input for ORIGEN.

The MCNP modeling was run for 10^8 neutron histories with the results tabulated for each location and converted to inputs for ORIGEN. This provides a first estimate of the nuclide specific activities for the entire 6-month operation.

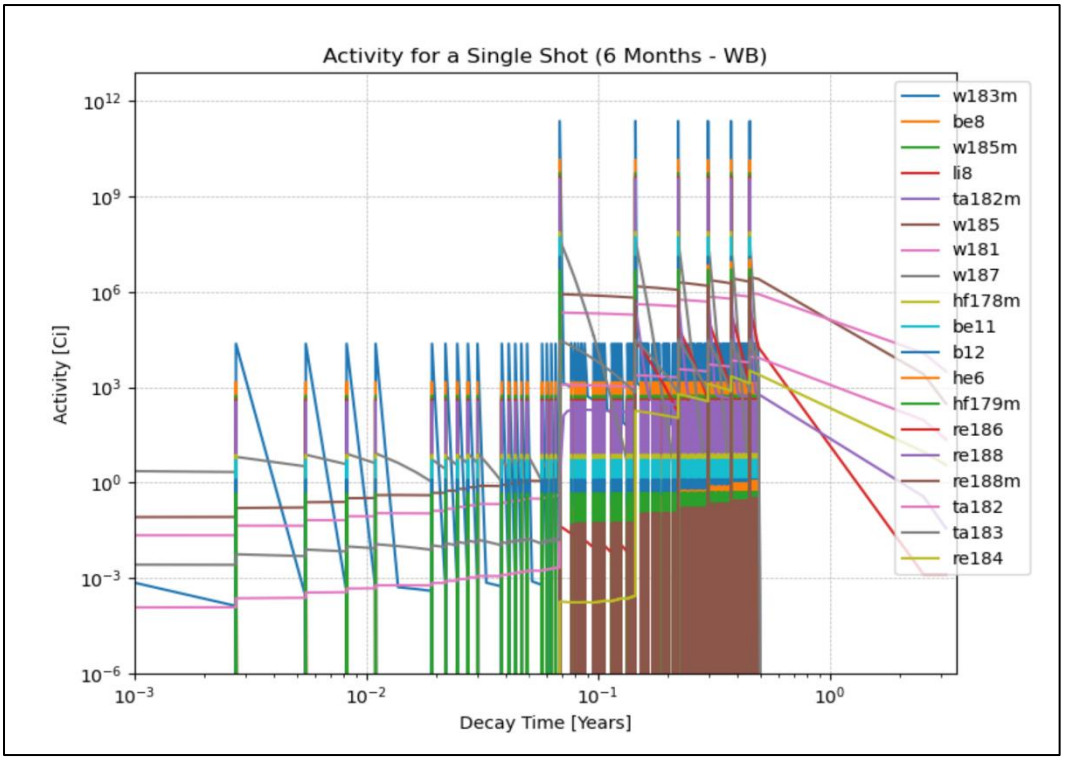

Figure 5: Isotopic activities for WB - Natural Boron-10 concentrations over a 6-month cyclical activation period with 2 years of decay at (0, 618, 0).

From this, the dominant species are W-183m and Be-8, however these die off relatively soon after a shot occurs. One of the most impressive features of this program is that it shows the buildup of otherwise unsuspected isotopes. For example, initially lithium-8 is not a concern. As soon as the first high yield neutron shot is complete lithium-8 begins to build-up to non-negligible values. This is seen for many isotopes, including W-181 which dominates after the 6-month irradiation cycle. It is entirely possible that longer irradiation times will enable more isotopes to become dominant at later times and will be the focus of future studies. Furthermore, this enables us to compare with activation limits for Low-Level and High-Level wastes that have been set by the Nuclear Regulatory Committee and other local governing bodies. Another interesting view is that of the nuclide atom densities, in which stable isotopes are also shown. This can be of interest to material science studies in order to see the build-up of non-native elements. One example of this is inert gases which cause stress on materials.

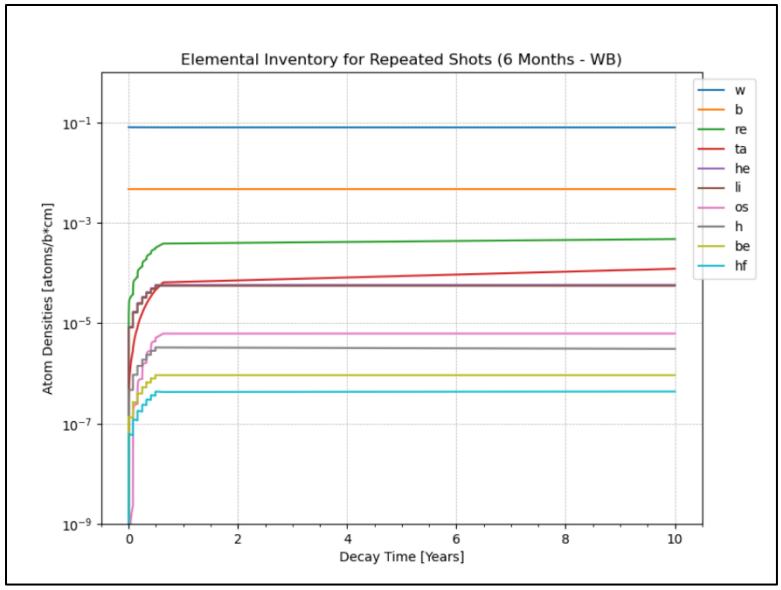

Figure 6: Atom densities for the 10 most dominant species during a 6-Month irradiation time on a WB, Natural B-10, sample at (0, 618, 0).

In these results, the buildup of these gases is seen such as helium and hydrogen. Helium accumulation along grain boundaries is a common issue in tungsten materials and may cause swelling in the material which should be studied. This could cause premature fracturing of material as well as potential release of radioactive material. Another principal issue is the accumulation of deuterium and tritium in the material. These are both principal isotopes of concern for waste management and radiotoxicity in fusion systems.

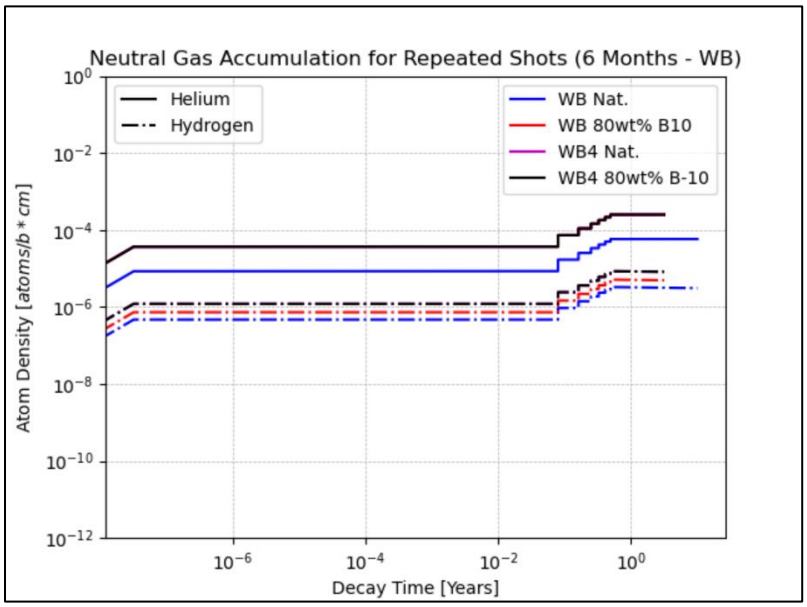

Figure 7: Comparison of helium and hydrogen accumulation in all WB compositions of interest during 6-Month irradiation and subsequent decay at (0, 618, 0).

One final aspect of the ORIGEN code which is very useful for these studies is the calculation of gamma rays over the time range and their matching gamma spectra. This is very convenient for looking at principal emitters of gammas and their matching energies for dose calculations. The program allows the user to specify time points in which the gamma spectra calculation is desired. It is then possible to plot each gamma spectra near each other and compare. This will be very useful in future dissertation work, in which samples of manufactured tungsten borides will be irradiated in fusion neutron environments. The irradiated samples will then be analyzed with a gamma spectrometer to compare the experimental results with the computational results provided by ORIGEN. This will provide a benchmark for understanding the program's effectiveness in predicting dose for planned operation of the facility.

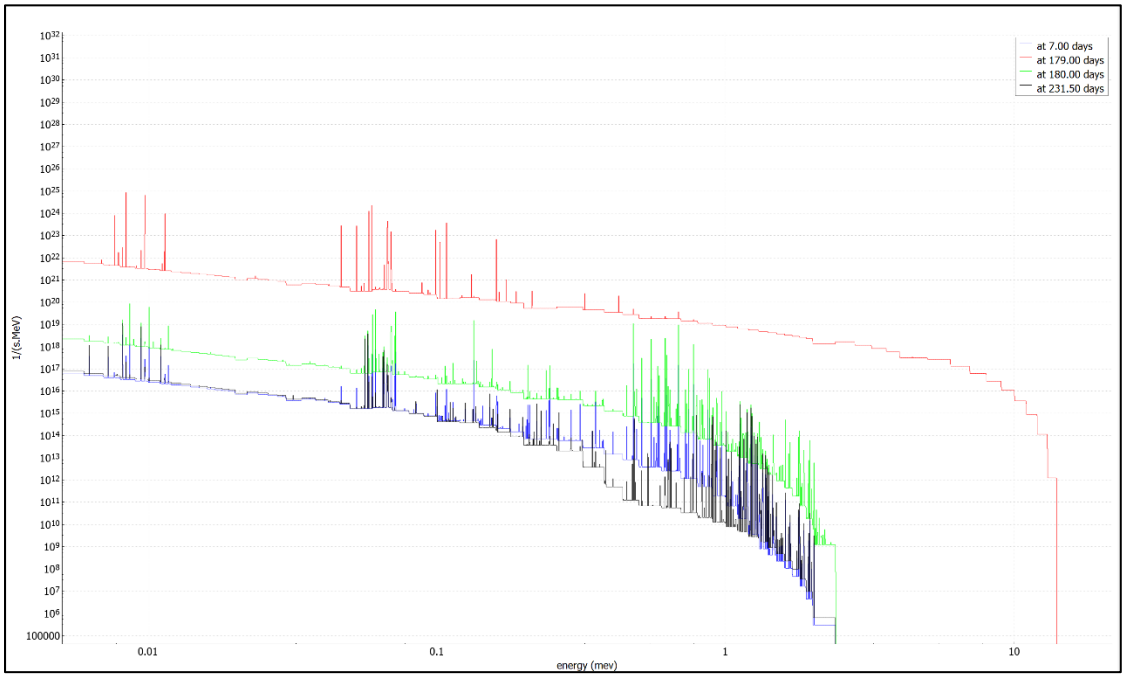

Figure 8: Gamma spectra for WB - Natural Boron-10 concentration at various time points during the solution time period at (0, 618, 0).

Conclusion

ORIGEN is a transmutation analysis program within the SCALE package from Oak Ridge National Laboratory. It has been shown that the program can provide a lot of useful insight to how radiation fields change the composition of a material over time. In specific this code is very useful for tracking the inventories of isotopes generated by the irradiation of a target material with complex scheduling. In this case, the system was operated daily for one second

with a yield of 10^{14} neutrons and once a month with a neutron yield of 10^{21} neutrons. It was found that the nano-second time scale solutions did not produce physically sound results and will need to be addressed in future studies to produce accurate isotopic inventories. The results from this program will be very useful, however, for analyzing many different questions that naturally arise in radiation environments. This includes the change in material composition and lattice structure, buildup of radioactive daughter products, accumulation of gaseous products and other concerns. This data will then enable engineers to develop shielding which limits dose to personnel and equipment while also being able deal with radioactive waste effectively when disposed.

References

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2. https://scale-manual.ornl.gov/origen/origen-theory.html
3. https://www-nds.iaea.org/exfor/servlet/E4sMakeE4

Acknowledgments

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