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**Idaho National Laboratory
Idaho Falls, Idaho 83415**

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Implementation of Depletion Architecture in the MAMMOTH Reactor Physics Application

Olin W. Calvin[†], Javier Ortensi[‡], and Yaqi Wang[‡]

[†]Nuclear Engineering Program, University of Florida

[‡]Department of Reactor Physics, Idaho National Laboratory



What is Depletion?

Depletion is the process by which the composition of a material changing as a result of radioactive decay or interactions with particles, such as neutrons. Currently operating nuclear reactors rely on neutrons to produce fission events (which release usable energy) in isotopes such as uranium-235. As a result, uranium-235 is constantly being destroyed in nuclear reactors and replaced with fission products, with products such as xenon-135 having detrimental effects on the ability to sustain a fission chain reaction. Thus accurate modeling of depletion is critical to developing safe, reliable, and efficient nuclear systems.

Architecture

Point-wise depletion is currently implemented in MAMMOTH. In a finite-element method framework, such as MOOSE [3, 2], this can take many forms. While the initial implementation supported quadrature point and element-wise depletion, this now includes predefined depletion zones identified via a variable (depletion ID) included in the FEM mesh. This allows users the ability to freely define spatial depletion zones with any level of complexity and provides the ability to include many elements in a single depletion zone thereby reducing computational expense and allowing calculations in significantly larger domains [1].

A new decay data format, known as ISOXML, was developed in order to handle the decay data for isotopes, since cross-section data handling was already implemented. ISOXML takes advantage of the fact that the ISOXML format is both machine and human readable. The Oak Ridge Isotope Generation application [4] utilizes one of the most extensive decay data libraries built from the ENDF data set in order to track the radioactive decay properties of over 1,600 nuclides, significantly more than the original MAMMOTH dataset of 300. In order to use this data, a reader was implemented into MAMMOTH to convert this data into the ISOXML format used by MAMMOTH. A comparison of the ISOXML and ORIGEN formats are shown in Figures 1 and 2.

```
<isotope Name="MO96" Z=42 A=96 DecayConstant="4.81352286722194208e-06">
  <DecayTypes>Beta DoubleBeta Neutron BetaAlpha</DecayTypes>
  <DecayEnergies>2.67900000e+00 2.67900000e+00 2.67900000e+00 2.67900000e+00</DecayEnergies>
  <DecayGammaEnergyFractions>0.00000000e+00 0.00000000e+00 0.00000000e+00 0.00000000e+00</DecayGammaEnergyFractions>
  <DecayBranchingRatios>6.50000000e-01 1.50000000e-01 1.00000000e-01 1.00000000e-01</DecayBranchingRatios>
  <DecayDaughters>TC96 RU96 MO95 MO92</DecayDaughters>
</isotope>
```

Fig. 1: Non-physical ISOXML decay data entry for Molybdenum-96.

1	420960	3	4.0000E+01	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1			0.0000E+00	0.0000E+00	2.6790E+00	1.0000E+01	1.0000E+00	1.0000E+00	0.0000E+00
1			0.0000E+00	6.5000E-01	1.5000E-01	1.0000E-01	1.0000E-01		

Fig. 2: Non-physical ORIGEN decay data entry for Molybdenum-96.

DRAGON-5 Comparison

In order to demonstrate the correctness of the depletion implementation in MAMMOTH, a comparison between DRAGON-5 [5], a depletion application maintained by the Ecole Polytechnique de Montreal, and MAMMOTH was performed. The input was a homogenized pressurized water reactor fuel cell exposed to a constant flux for 600 days with 297 isotopes tracked. The results of the relative difference in final concentrations for select isotopes as well as the results of eigenvalue calculations are shown in Figures 3 and 4 and indicate significant agreement between DRAGON-5 and MAMMOTH which is within the precision of the data used by DRAGON-5.

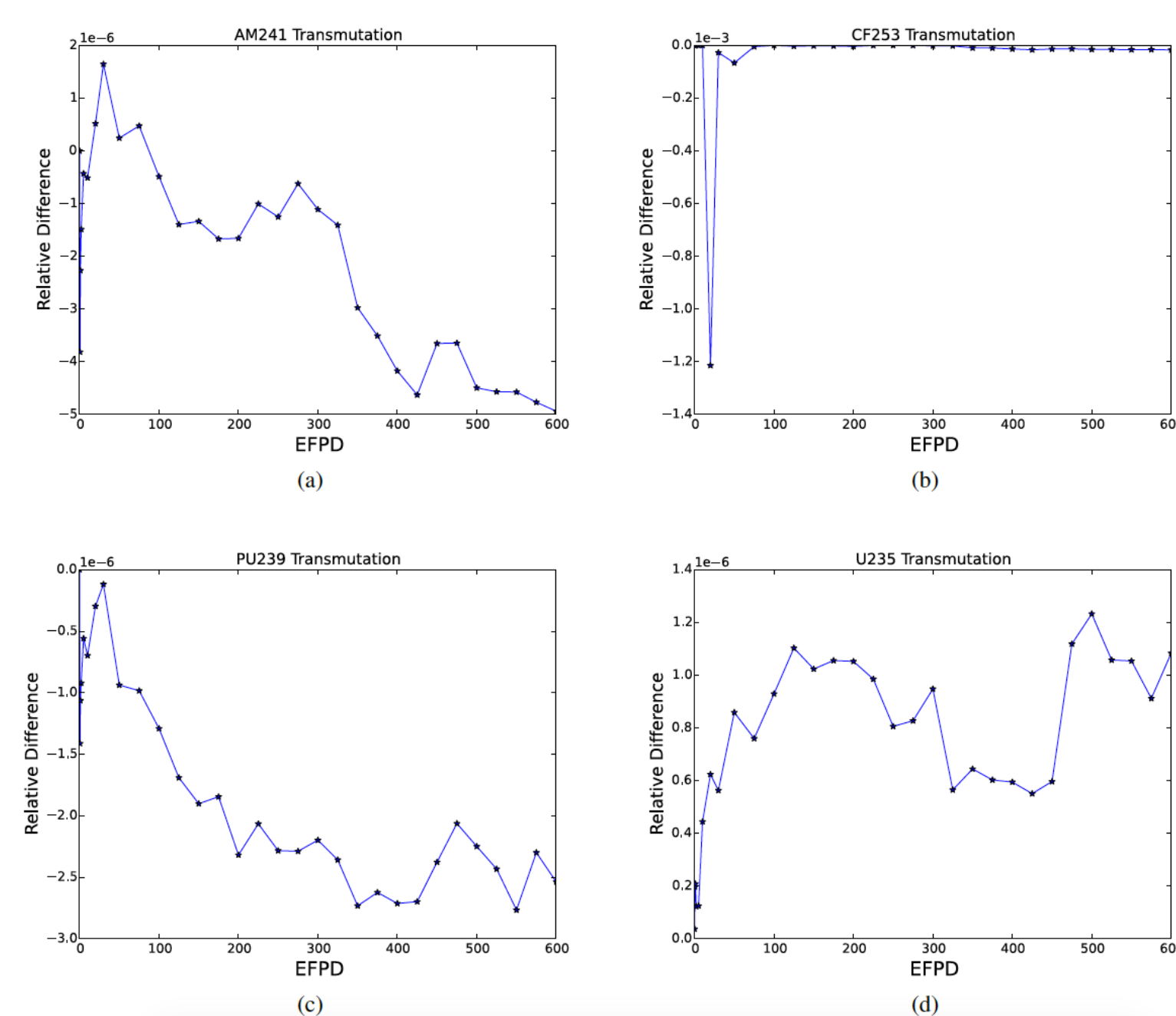


Fig. 3: Relative differences between DRAGON-5 and MAMMOTH number density solutions for (a) Americium-241, (b) Californium-253, (c) Plutonium-239, (d) Uranium-235.

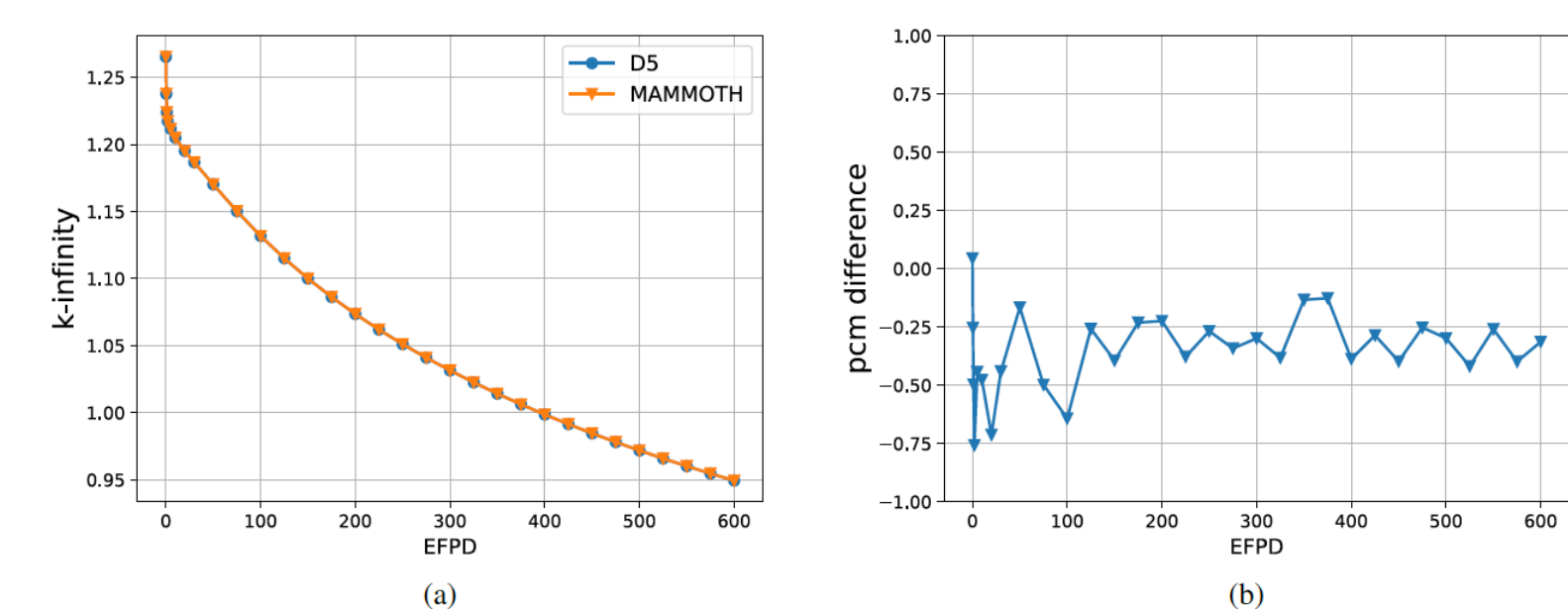


Fig. 4: (a) Eigenvalue results from DRAGON-5 and MAMMOTH, (b) Per cent mille difference between DRAGON-5 and MAMMOTH.

ORIGEN Comparison

In order to test the ability of MAMMOTH to perform constant power depletion, a comparison was made between ORIGEN and MAMMOTH for the depletion of a sample nuclear fuel at 30 MW for 1100 days, to achieve a total burnup 33 GWd/MTU. Over 1,400 isotopes were tracked during the calculation with the relative difference in the number densities of xenon-135, plutonium-239, and uranium-235 shown in Figures 5 through 7 as these isotopes have significant effects on nuclear systems. In addition, plutonium and xenon demonstrated large relative differences. Upon further research, these differences are considered to be a result of approximations and simplifications made by ORIGEN in order to speed up calculations while MAMMOTH does not make these simplifications.

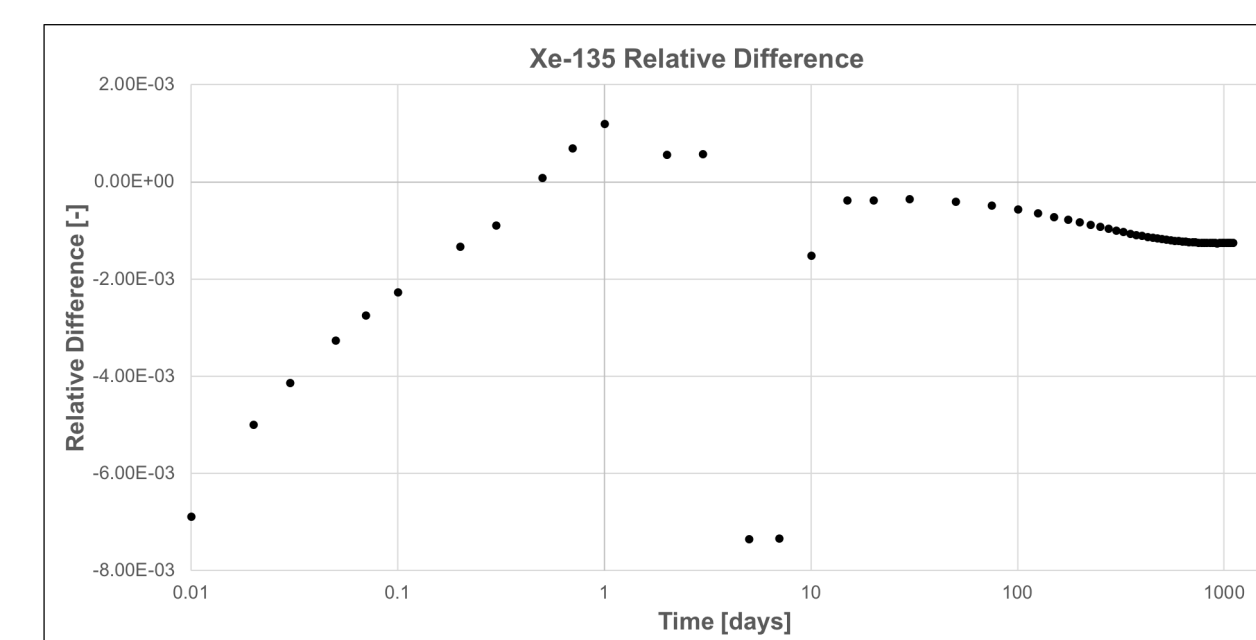


Fig. 5: Relative difference between ORIGEN and MAMMOTH number density solutions for Xenon-135.

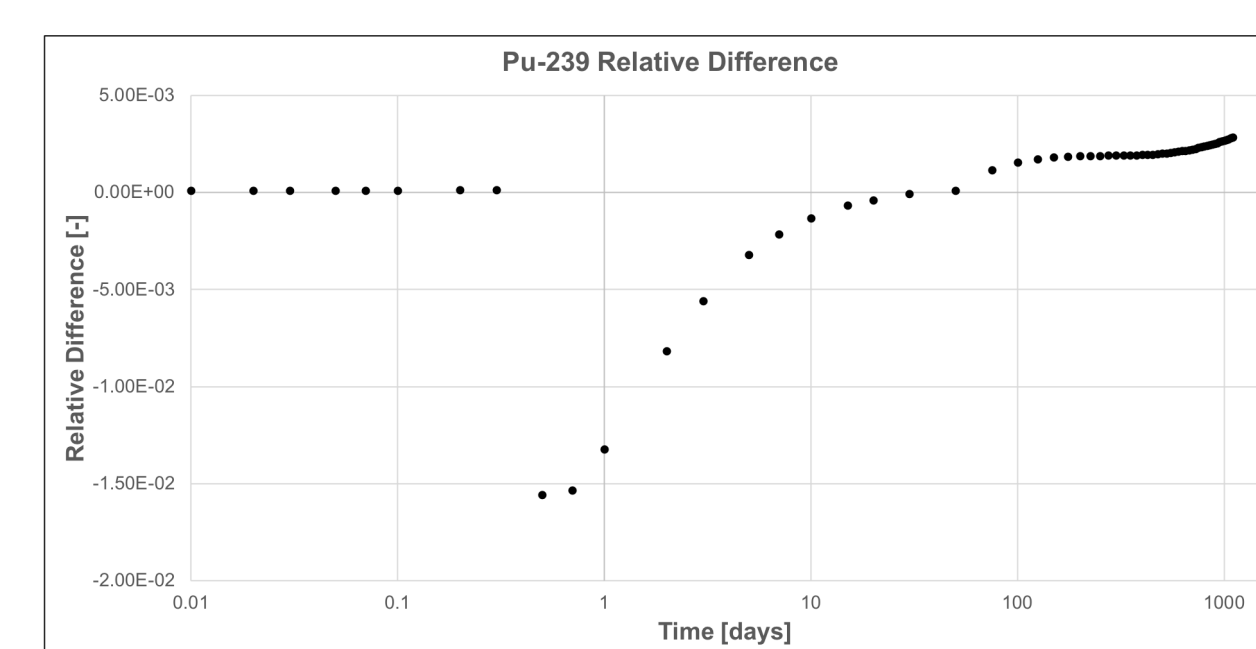


Fig. 6: Relative difference between ORIGEN and MAMMOTH number density solutions for Plutonium-239.

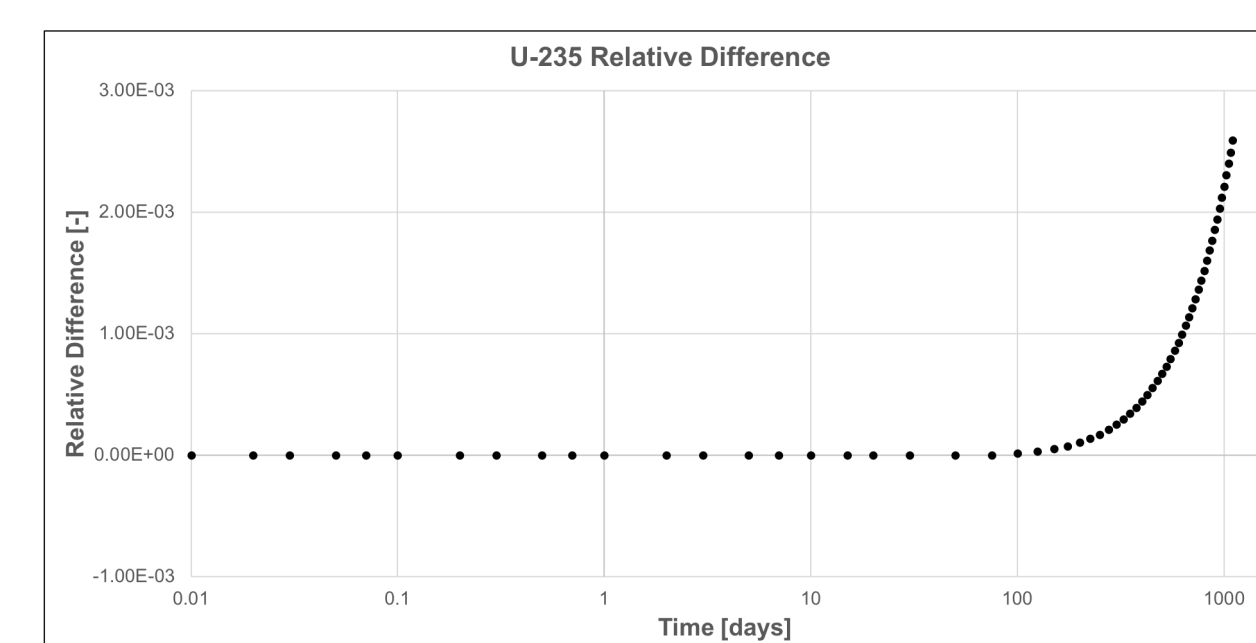


Fig. 7: Relative difference between ORIGEN and MAMMOTH number density solutions for Uranium-235.

Conclusion

The depletion architecture in MAMMOTH has been modified to improve both user flexibility in performing depletion calculations through the addition of depletion ID specification and developer flexibility in future development of MAMMOTH as its mission statement continues to evolve. These modifications have been verified against both computational benchmark problems and in code-to-code comparisons with ORIGEN and DRAGON-5. The functionality to track thousands of isotopes, which is required for the ORIGEN data set, has been implemented, improving upon the original implementation using hundreds of isotopes. The ISOXML format for storing decay and transmutation data within MAMMOTH has been developed providing a format which is human and machine readable.

Future work will include:

- the implementation of a predictor-corrector method for constant power problems to improve the numerical accuracy of constant power depletion calculations without significant increases in computational expense and
- the performance of validation studies against experimental measurements such as those from the Advanced Test Reactor (ATR).

References

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