INL/CON-19-55641-Revision-0

Implementation of Depletion Architecture in the MAMMOTH Reactor Physics Application

August 2019

Changing the World's Energy Future

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Idaho National Laboratory

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

Implementation of Depletion Architecture in the MAMMOTH Reactor Physics Application

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Introduction

- Goal is to add functionality to MAMMOTH to perform depletion calculations. The purpose of this is to allow the use of the same mesh for fuel elements depleted in commercial reactors or the Advanced Test Reactor (ATR) before being placed in the Transient Reactor Test Facility (TREAT) for further experimentation.
- Easily extendable and modifiable data sets are also desired as new and more accurate and/or more applicable cross section and decay data becomes available.

Outline

Depletion

- Over time, the composition of materials in a nuclear reactor, particularly the fuel, changes as a result of both radioactive decay and neutron transmutation (fission, radiative capture, etc.)
- While the rate of radioactive decay relies on decay constants, neutron reaction rates can vary greatly over the lifetime of a reactor since they are dependent on cross sections and neutron flux.
    - Cross sections are dependent on temperature, incident neutron energy, etc.
    - Neutron flux varies over time in a reactor as the flux typically needs to increase over time in order to maintain a constant power level as the fuel is depleted.

The Bateman Equations

- The analytic solution to decay rates for radioactive isotopes was developed by Harry Bateman[1].
- The Bateman equation for the decay of uranium-238 is shown below where λ_{U238} is the decay constant for uranium-238:

$$\frac{dN_{U238}(t)}{dt} = -\lambda_{U238} N_{U238}(t)$$

- The Bateman equation can then be extended to include loss or gain of a given isotope as a result of neutron transmutation.
- The Bateman equation for the change in number density of uranium-238 when taking into account both radioactive decay and neutron absorption events as a result of a monoenergetic neutron flux (ϕ) with a constant absorption cross-section ($\sigma_{a,U238}$) is shown:

$$\frac{dN_{U238}(t)}{dt} = -\lambda_{U238} N_{U238}(t) - \phi\sigma_{a,U238} N_{U238}(t)$$

[1] H. Bateman, "Solution of a system of differential equations occurring in the theory of radioactive transformations," (1910).

The Depletion Matrix

- In a typical reactor system, you will have hundreds of isotopes simply because of the isotopes which can be generated as a result of nuclear fission.
- The Bateman equations can be merged into a matrix which can then be solved using a variety of methods.
- Assuming we have a system tracking iodine-135, xenon-135, and xenon-136, all of which are subjected to a neutron flux, we can obtain the following Bateman Equations, assuming the cross sections for iodine-135 and xenon-136 is negligible compared to the xenon-135 cross section.

$$\frac{dN_{Xe136}}{dt} = \phi\sigma_{a,Xe135}N_{Xe135}$$

$$\frac{dN_{I135}}{dt} = -\lambda_{I135}N_{I135}$$

$$\frac{dN_{Xe135}}{dt} = -\lambda_{Xe135}N_{Xe135} - \phi\sigma_{Xe135}N_{Xe135} + \lambda_{I135}N_{I135}$$

The Depletion Matrix

- Each production and loss term can be grouped together for each isotope in a matrix with the number densities placed in a separate vector.
- Notice that the decay product of Xenon-135 is not accounted for in this system, meaning over time there will be a decrease in the total atomic number density of our system as the decay product Cs-135 is ignored.

$$\begin{bmatrix} 0.0 & 0.0 & \phi\sigma_{a,Xe135} \\ 0.0 & -\lambda_{I135} & 0.0 \\ 0.0 & \lambda_{I135} & -\lambda_{Xe135} - \phi\sigma_{a,Xe135} \end{bmatrix}$$

Data Loader

- Functionality to read ORIGEN-formatted ENDF decay data added.
- The ISOXML format was developed for storing the decay data. XML format was chosen because it is both human and machine readable and can be easily modified/extended as needed.

Data Loader

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

Example ORIGEN decay data entry for molybdenum-96


```
<Isotope Name="MO96" ZAID="420960" DecayConstant="4.81352208722184208e-06">
  <DecayTypes>Betam DoubleBetam Neutron BetamAlpha</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 NB92</DecayDaughters>
</Isotope>
```


Example ISOXML decay data entry for molybdenum-96

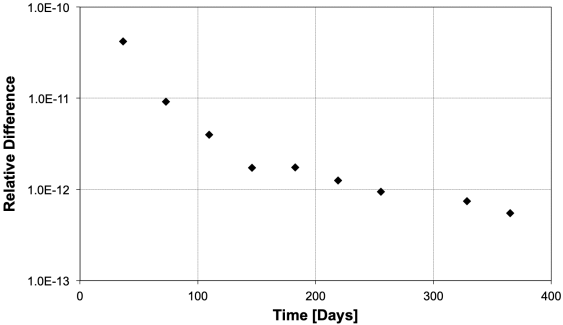
Architecture Improvements

- Significant effort was spent reworking the previous depletion implementation in MAMMOTH to take advantage of the MOOSE framework namely for time step execution and depletion zone specification.
- The Chebyshev Rational Approximation Method[2] (CRAM) is used to calculate the new number densities after each subsequent time step.
- This new implementation was tested for several different problems.

[2] M. Pusa, "Rational Approximations to the Matrix Exponential in Burnup Calculations," (2011).

Thorium Benchmark

- A reference benchmark solution for the decay of thorium-232 for one year is available[3].



Relative error between the MAMMOTH and reference solutions for lead-208

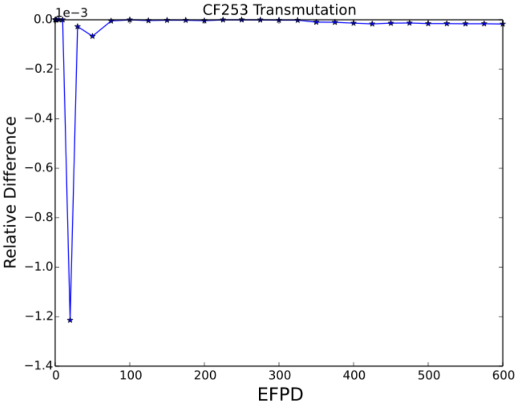
[3] K. Huang, Y. Li, and B. Ganapol, "A Backward Euler Doubling Feasibility Study Based on Thorium Series Cascade," (2016).

DRAGON5 Comparison

- A homogenized PWR fuel pin was subjected to constant one energy group neutron flux irradiation for 600 days and the results from MAMMOTH compared to those from DRAGON5[4].
- The DRAGON5 data set was used in this calculation and a total of 297 isotopes were tracked in the system.

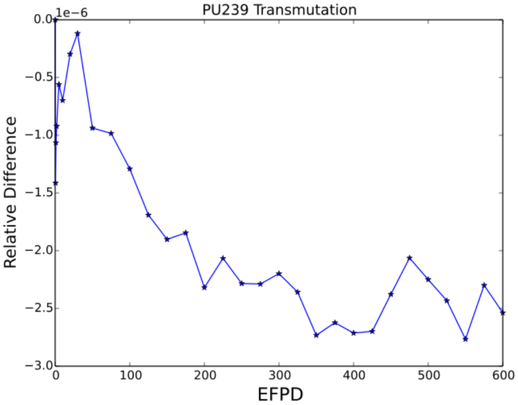
[4] G. Marleau, A. Hebert, and R. Roy, "A User Guide for DRAGON Version 5," (2018).

DRAGON5 Comparison



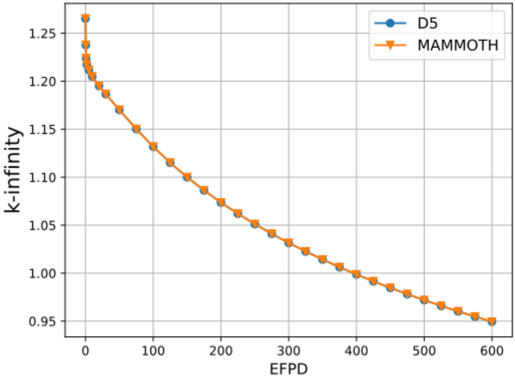
Relative difference between solutions for californium-253

DRAGON5 Comparison



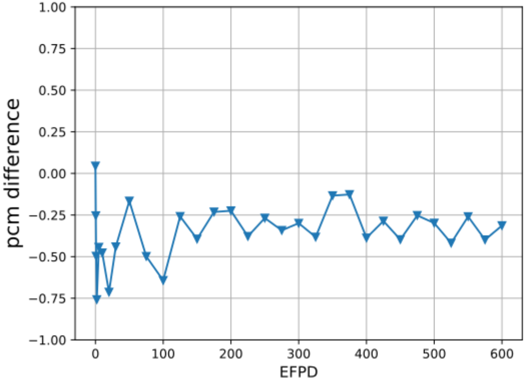
Relative difference between solutions for plutonium-239

DRAGON5 Comparison



Eigenvalue results for MAMMOTH and DRAGON5

DRAGON5 Comparison

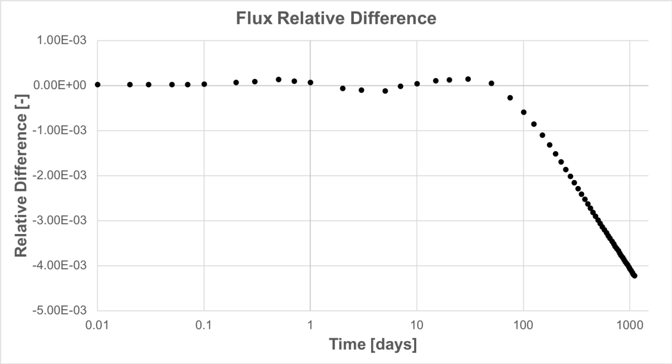


Per cent mille differnece between MAMMOTH and DRAGON5

ORIGEN Comparison

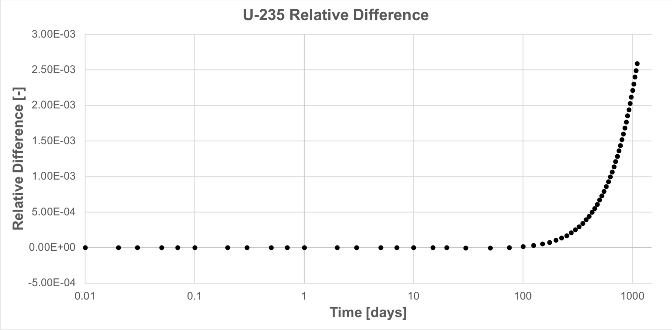
- In order to test constant power depletion capabilities of MAMMOTH a comparison was made to ORIGEN.
- A metric ton of 5% enriched uranium was depleted at rate of 30 MW for 1,100 days for a total burnup of 33 GWd/MTU.
- Over 1,400 isotopes were tracked in the system.

ORIGEN Comparison



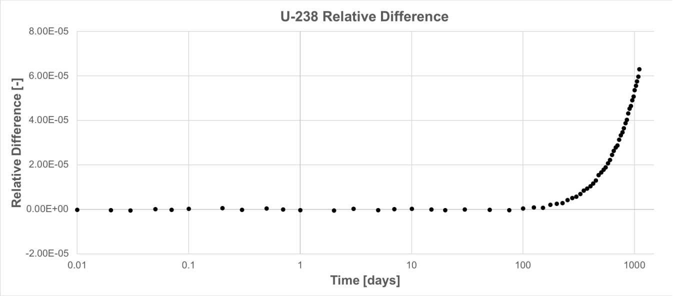
Relative difference for neutron flux between ORIGEN and MAMMOTH

ORIGEN Comparison



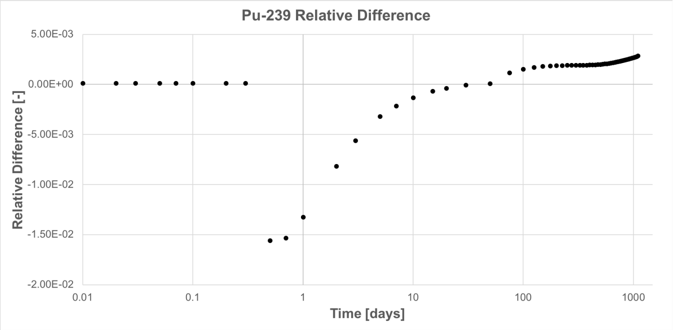
Relative difference for uranium-235 between ORIGEN and MAMMOTH

ORIGEN Comparison



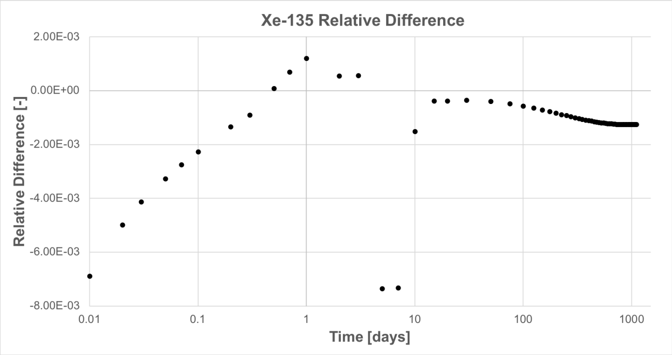
Relative difference for uranium-238 between ORIGEN and MAMMOTH

ORIGEN Comparison



Relative difference for plutonium-239 between ORIGEN and MAMMOTH

ORIGEN Comparison



Relative difference for xenon-135 between ORIGEN and MAMMOTH

Summary

- Ability to process ORIGEN-formatted ENDF decay data has been added.
- Previous depletion implementation has been refactored and constant power depletion functionality has been implemented.
- Future Work:
  - Test multigroup depletion capabilities.
  - Implement predictor-corrector functionality for solving depletion problems.
  - Couple to RATTLESNAKE to deplete using the results of a neutron transport calculation and then use said results to do a subsequent neutron transport calculation.

Acknowledgements

The authors thank the staff of Idaho National Laboratory for their support of this work. This work was funded at INL under the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program managed by the Department of Energy Office of Nuclear Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

Questions?