Impact of Composition Approximation on Simulated Nuclear Fuel Cycle Metrics

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Objectives

Compare the validity and limits of simplifying Used Nuclear Fuel (UNF) composition by comparing high-resolution UNF inventory in 2020 from the UNF Storage, Transportation & Disposal Analysis Resource and Data System (UNF-ST&DARDS) [3] with a UNF inventory generated by assuming an average burnup and enrichment. We compare:

- Isotopic mass
- Waste management metric
- Equivalent ^{239}Pu Factor [2]

Introduction

UNF-ST&DARDS has been developed to integrate a centralized UNF database [3] and the SCALE suite of codes [1] to perform neutronics analysis for UNF management and disposal analysis. This comprehensive, high-resolution database lists every UNF assembly discharged in the U.S ($\sim 244,896$) and their properties (initial enrichment, burnup, ORIGEN-depleted isotopic composition, assembly type, etc.). While high resolution of this kind is exceptionally valuable, the volume of data can present challenges for processing and simulation computation times.

We compare the predicted U.S. UNF inventory in 2020 calculated using UNF-ST&DARDS to the same prediction calculated using a simplified UNF inventory assuming an average burnup and enrichment in order to assess the impact of this common simplifying assumption on fuel cycle metric accuracy.

Methods

We compare the predicted U.S. UNF inventory in 2020 calculated using UNF-ST&DARDS to the same prediction calculated using a simplified UNF inventory assuming an average burnup and enrichment in order to assess the impact of this common simplifying assumption on fuel cycle metric accuracy.

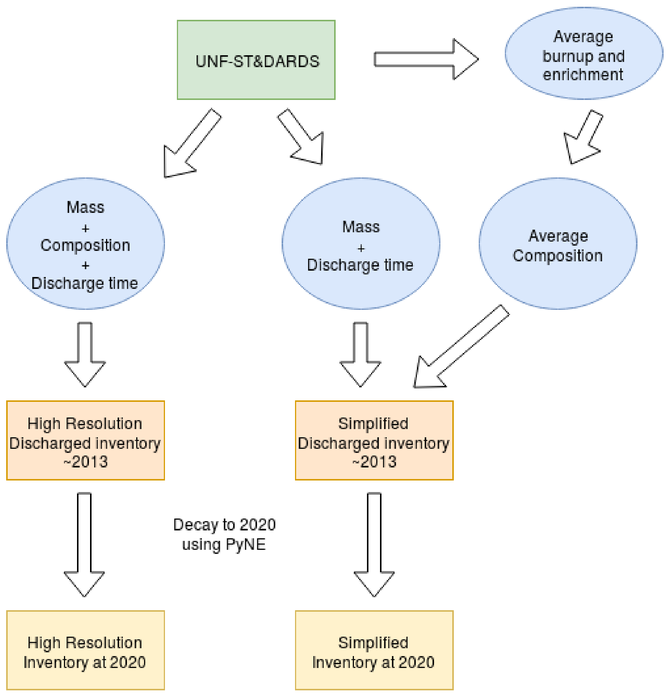

Figure: Workflow for generating two UNF inventories using UNF-ST&DARDS

Metrics

UNF is typically either destined for disposal (after storage) or reprocessing. Accordingly, the U.S. UNF inventory can be analyzed in two different ways, with certain metrics important for each.

Analysis type	Important metric	Unit
Fuel cycle analysis	Equivalent Pu-239 [2]	t
Waste management	Decay heat (@ 2020, 2100, 3100)	MW
	Activity (@ 2020, 2100, 3100)	Bq

Table: Important metrics for UNF with regard to analysis types

The relative difference values are calculated using the following formula:

$$\Delta M_i = M_{HR} - M_S$$

$$\text{Rel. Error} = \frac{M_{HR} - M_s}{M_{HR}}$$

M_{HR} = Metric in inventory (high-resolution case)

M_S = Metric in inventory (simplified case)

Average Composition

The average burnup of the assemblies in the Unified Database (UDB) was $36.169 GWD/MTHM$ and the average enrichment was $3.39\%^{235}U$. With these average values, we selected an assembly closest to the average.

Isotope	wt %
^{238}U	96.5000
^{235}U	1.0400
^{241}Am	0.0160
^{239}Pu	0.7550
^{137}Cs	0.1320
$90Sr$	0.0552
Pu Total	1.2760

Table: Composition of the representative assembly selected for analysis.

PyNE and ORIGEN Decay Calculation Comparison

To ensure the validity of the decay function implemented in Python for Nuclear Engineering (PyNE), we imported the database into PyNE and decayed each assembly to 2020.

Metric	PyNE	ORIGEN	Δ%
^{239}Pu mass [t]	520.52	520.50	3.8E-05
^{137}Cs mass [t]	59.23	59.19	6.7E-04
^{235}U mass [t]	771.42	771.39	3.8E-05
Total mass [t]	68,072	67,984	1.2E-03
Decay Heat [MW]	61.31	61.10	3.4E-03
Activity [Bq]	6.76e20	6.74e20	2.9E-03

Table: Comparison between PyNE decayed and ORIGEN decayed UNF inventory in 2020.

Isotopic Mass

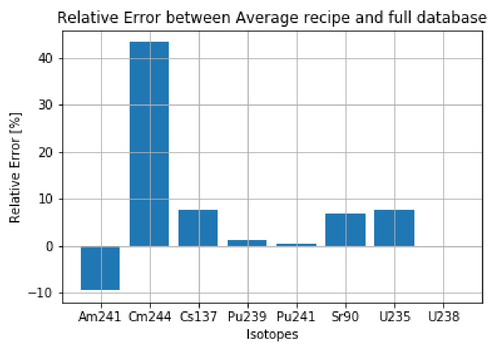

Figure: Relative error between high resolution and simplified case for different isotopes.

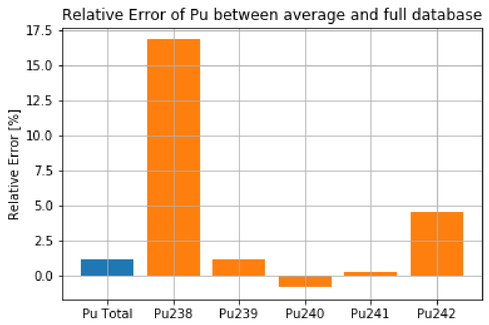

Figure: Relative error between high resolution and simplified case for plutonium isotopes.

Waste Management Metrics

The two major waste management metrics are radioactivity and decay heat. Since the two metrics change in time, the metrics are evaluated in time.

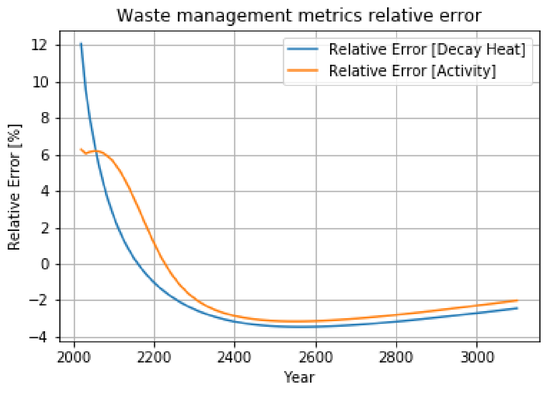

Figure: Relative error of activity and decay heat of the UNF inventory over time.

Fuel Cycle Analysis Metrics

Given the isotopic compositions of the UNF profile in 2020, we calculate the equivalent ^{239}Pu for both cases, for both spectra. The results are shown in Table 4. The figures show that the equivalent ^{239}Pu difference between two cases is 7% for thermal, and less than 5% for fast spectra.

Category	Equiv. ^{239}Pu ton	Rel. Error [%]
HR thermal	880.5	7.28
Simplified thermal	816.4	
HR fast	1214.0	4.67
Simplified fast	1157.3	

Table: Equivalent ^{239}Pu ton value comparison for High-resolution and simplified case.

To explain this error, we plotted every assembly and its normalized equivalent ^{239}Pu, shown in Figures 5 and 6. The normalized equivalent ^{239}Pu is simply the total equivalent ^{239}Pu divided by the total mass of the assembly.

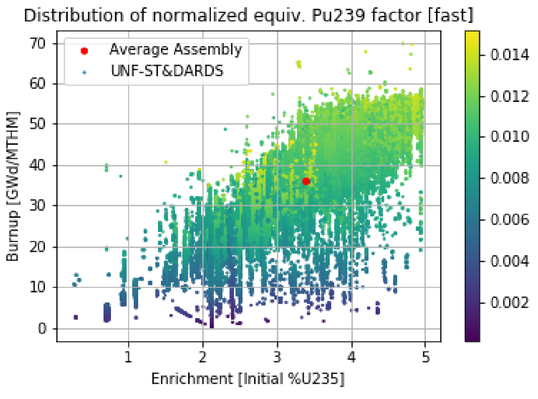

Figure: All assemblies in the database and their normalized equivalent Pu-239 in a fast reactor.

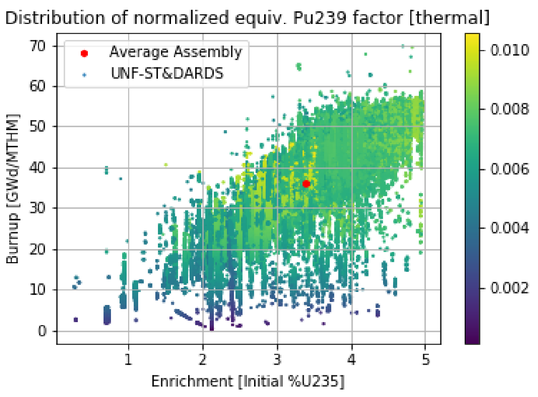

Figure: All assemblies in the database and their normalized equivalent Pu-239 in a thermal reactor.

Conclusion

We compared the simplified UNF inventory and the high-resolution UNF inventory at 2020 by calculating the isotopic differences as well as important metrics for waste management and fuel cycle analysis. Results show:

- Simplified inventory is **not adequate** for waste management analysis
  - Large error in FP and MA inventory
    - FP and MA sensitive to initial enrichment and burnup
    - FP and MA contributor in decay heat and activity
  - Discrete modeling for assemblies in repository modeling
- Simplified inventory is acceptable approximation for fuel cycle analysis
  - ~5% error for equivalent ^{239}Pu
  - Reduces computational burden for fuel cycle simulators

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