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Title: Recent Advances in Monte Carlo Burnup Calculations for PWR Used Fuel Libraries

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Abstract

The Next Generation Safeguards Initiative (NGSI) of the U.S. Department of Energy (DOE) has funded a multilaboratory/university collaboration to quantify the plutonium (Pu) mass in, and to detect the diversion of pins from, spent nuclear fuel assemblies. Developing an accurate representation of spent nuclear fuel is an important component of assessing detector models for nondestructive assay (NDA) techniques. Excluding oxygen, spent nuclear fuel consists of about 94–96 wt% U, 1 wt% Pu and minor actinides, and 3–5 wt% fission products. This presentation describes three different spent fuel libraries that have been or will be created for the NGSI effort to represent a range of material compositions present in Pressurized Water Reactor (PWR) spent fuel assemblies. The first library involved an infinitely-reflected assembly calculation with four radial regions, the second library yields results for a more realistic, asymmetric burn calculation with only one radial region, and the third library will give results of sensitivity analyses on the first two. The presentation also displays results of benchmark calculations for PWRs that have been examined using destructive analyses.

Recent Advances in Monte Carlo Burnup Calculations for PWR Used Fuel Libraries

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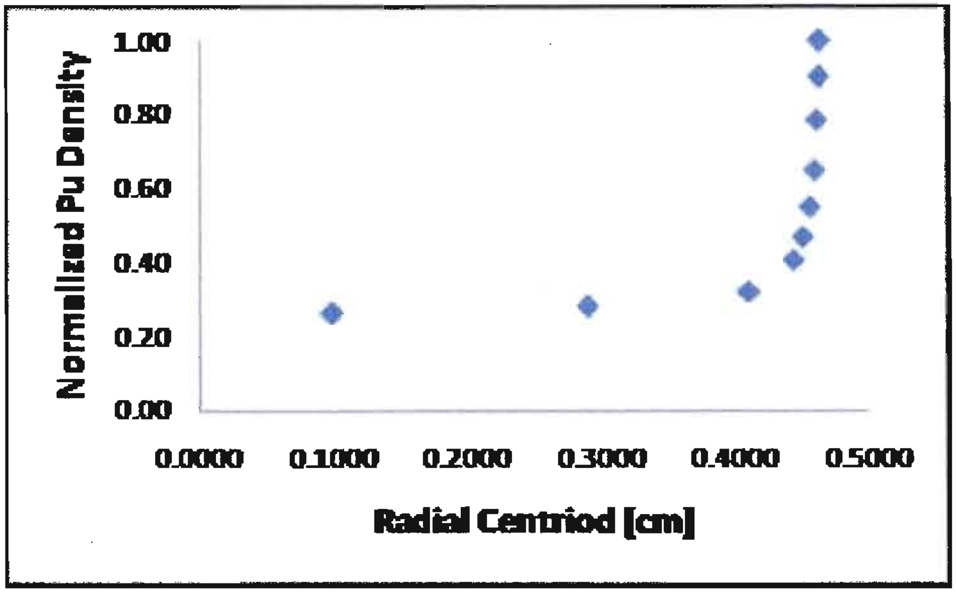
Introduction

- Many burnup codes exist worldwide, but few offer the advantage of the flexibility present in the Monte Carlo transport code MCNP/X.
- Increases in computational power are making MCNP/X simulations of a full reactor core more feasible.
- Memory restrictions in MCNP/X have limited detailed burnup calculations to 100-200 material regions in the past (based on geometry and available RAM).
- Option to reduce memory requirements in MCNPX Version 2.7.0 now exists.
- *Monteburns* links calculations from MCNP/X and depletion code CINDER90 or ORIGEN-S for up to 495 (soon more) burn materials and now performs parallel depletion calculations.
- Burning thousands of individual regions (such as every pin in a PWR core) is still challenging but forthcoming in the near future.

NGSI Program

- Next Generation Safeguards Initiative goal is to develop an instrument capable of determining plutonium (Pu) mass in used fuel assemblies.
- MCNPX was chosen to design instruments for NGSI because of its flexibility – MCNPX can track particle interactions at a wide variety of energies and geometries.
- To limit scope of the NGSI project, only Pressurized Water Reactor assemblies are modeled.
- If modeled appropriately, MCNPX depicts details of Pu buildup at the edge of a pin, important for some techniques.



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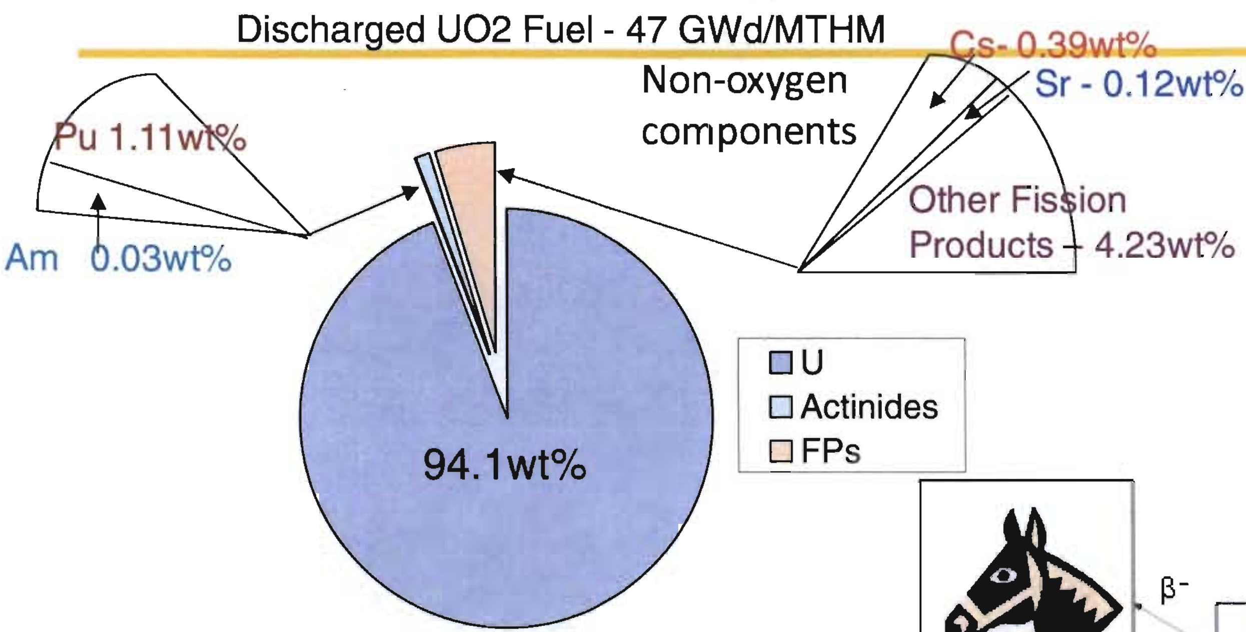
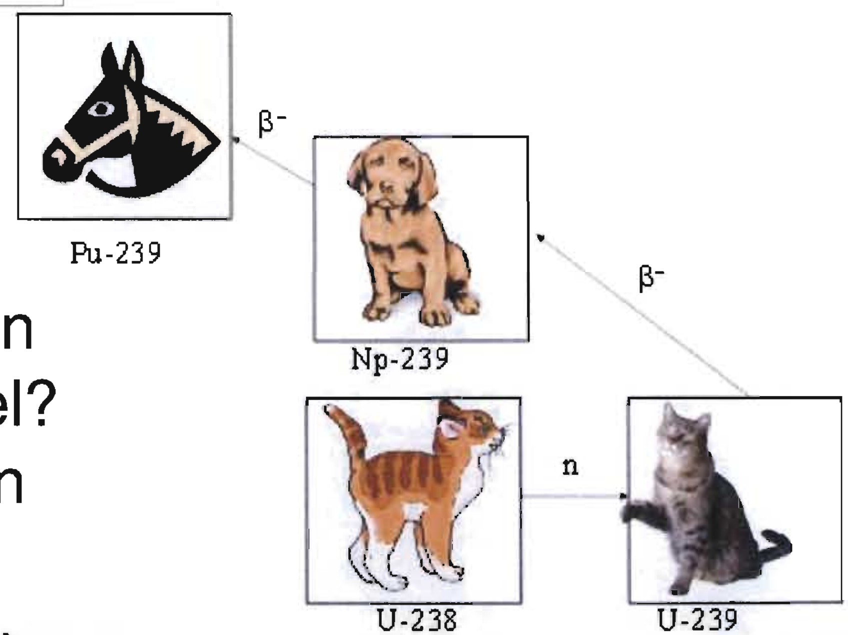
What does Used Fuel Comprise?





How Do Materials Other Than Uranium End up in Spent Fuel?
The Answer is Transmutation

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Libraries Created for NGSI Program

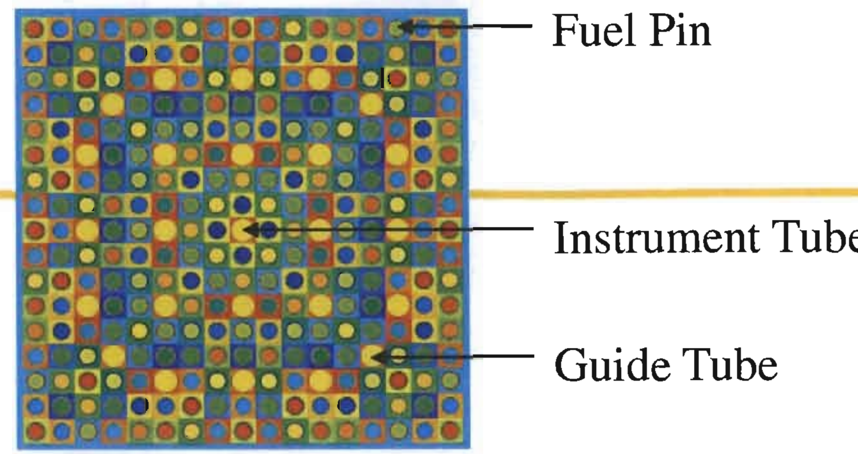
Three spent fuel libraries contain a range of burnups (BU) and conditions.

1. Infinitely-reflected assembly calculations last year with 4 radial fuel regions and as much fidelity as possible at the time.
2. "Representative" shuffled assembly tracked through PWR this year with 1 radial region.
3. Sensitivity study on various parameters for 4wt% initial enrichment (IE): shuffling scheme, temperatures, addition of control rods/burnable poisons, etc. is forthcoming.

IE/BU	2wt%	3wt%	4wt%	5wt%
15 GWd/MTU	X X	X X	X X X	X X
30 GWd/MTU	X X	X X	X X X	X X
45 GWd/MTU	X	X	X X X	X X
60 GWd/MTU	X	X	X	X X

X = Library #1
X = Library #2
X = Library #3

Library #1



- Infinitely-reflected generic 17 X 17 PWR; 39 rods symmetrically modeled in 1/8 of an assembly.
  - UO_2 fuel; Zircaloy-4 clad; no gap
  - Axially homogenous
- Dimensions obtained from OECD/NEA IVB Benchmark
- 4 Radial zones per pin: 0.39, 0.402, 0.4075, and 0.41 cm.
- ~2 GWD/MTU time durations after Xe and Sm equilibrium
- 1 and 4 weeks, 1, 2, 5, 20, 80 year cooling times (only red ones released)
- 10000 par/cycle; 155 cycles; skip 25 cycles
- Water density was 0.7245 g/cc.
- MCNPX in-line burnup capability used (i.e. CINDER90) with Tier 2 Fission Products (~80 Isotopes) .
- Fuel was at a temperature of 900 K and density of ~10.45 g/cc.
- Average boron concentration in water was 660 ppm; 575 K Water Temp.
- 600 K Cladding and Water Cross Sections were used.

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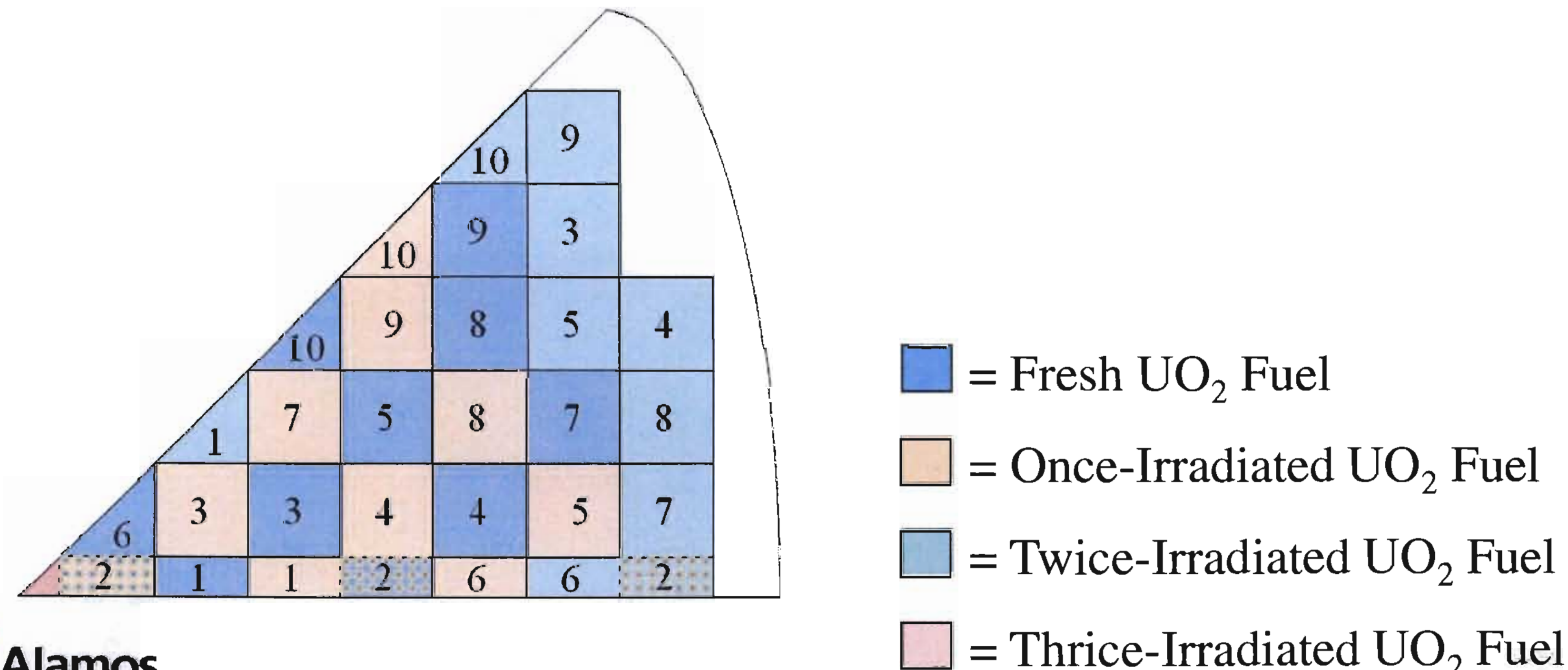
Library #2

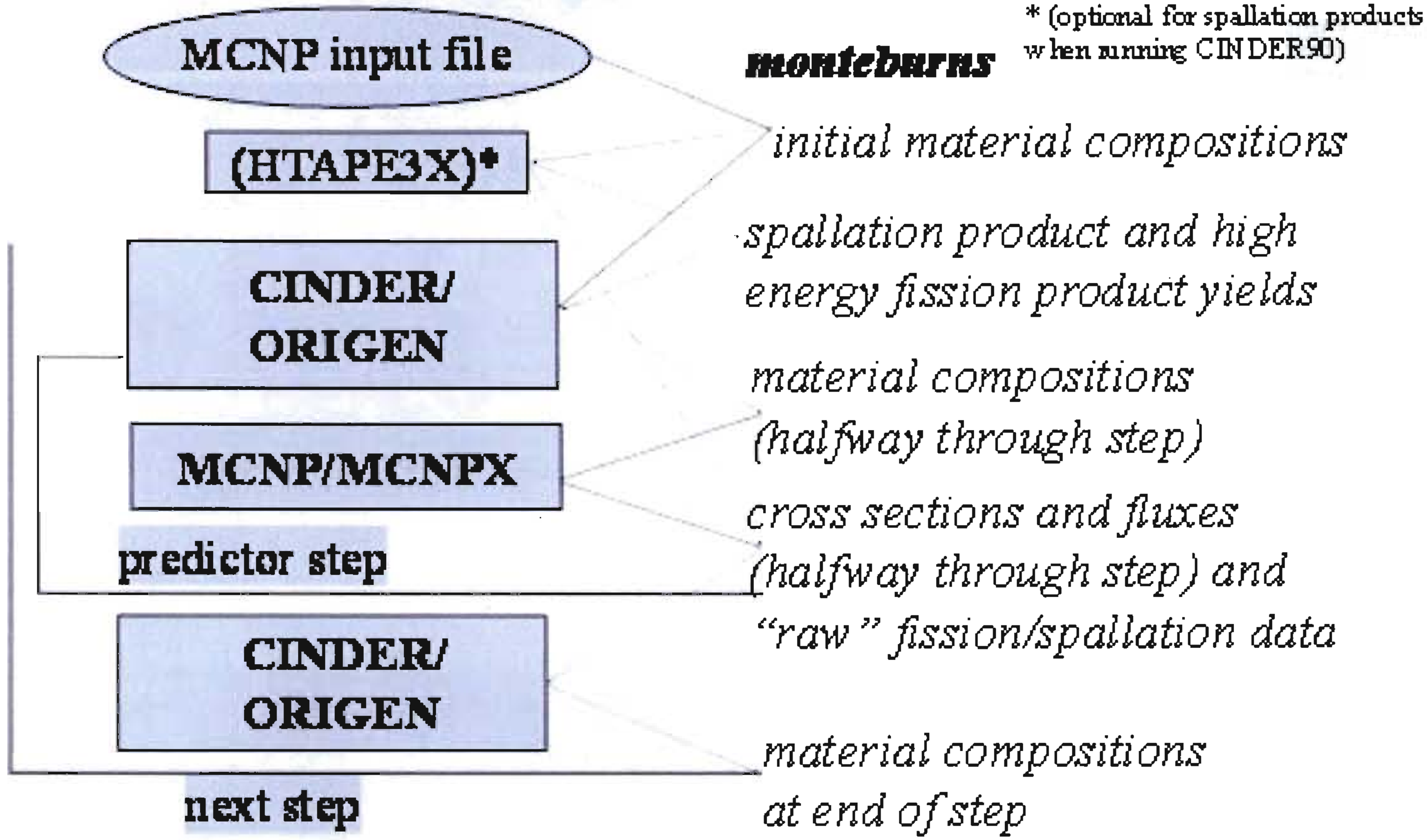
- Asymmetric burn of assembly performed using a 1/8 core reflected core model and 443 separate materials in *Monteburns* (only ~50 used in past).
- *Monteburns* is used with CINDER90; same premise as MCNPX burnup, just different linkage tool capable of core shuffling.
- Includes ^{234}U enrichment as well as ^{235}U.
- Includes 99.9 % of fission product mass (most included as "importance fraction" in *Monteburns*: significant contribution to absorption, fission, mass, or atom fraction).
- Gap was added, and boron concentration was reduced by ½ at a midpoint.
- Reduced number of IE/BU cases but only 1 radial region.
- CTs of 14 days, 1 yr, 5 yr, 20 yr, 40 yr, and 80 yr.
- Length of irradiation time step was tested and same answers were obtained for 40 vs. 80 days, so up to 80 day time steps were used.
- 400000 particles/cycle, 100 active cycles, 20 skipped cycles, and source files passed from one step to the next for best starting distribution.

Shuffling Scheme

- Each pin in the #2 assemblies is modeled as a separate burnup region (reflected ½ assembly);
- All pins in other assemblies are modeled separately for transport but are burned as one region.



Monteburns Flow Chart



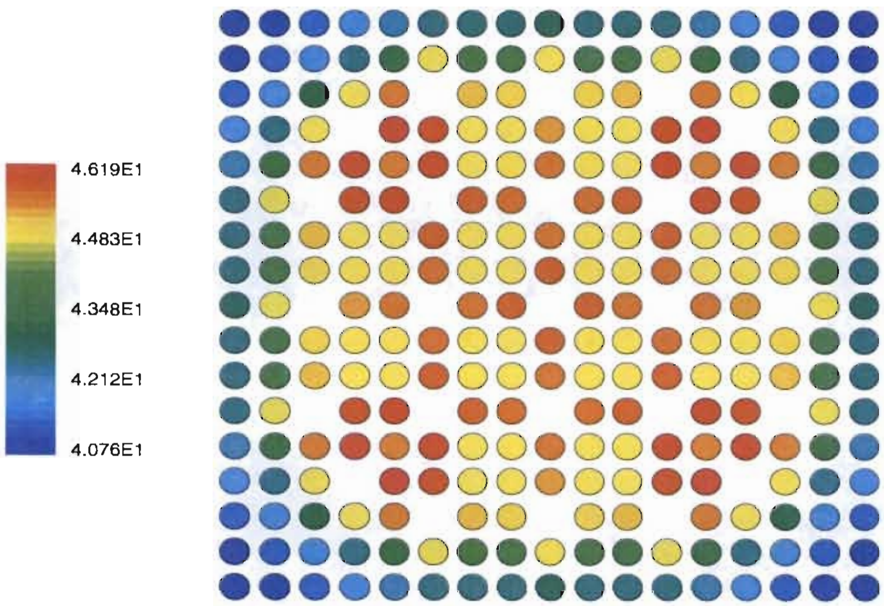
Monte Carlo burnup techniques (MCNPX, *Monteburns*) were designed to look at a range of reactor designs but can also be used to model a LWR! The amount of fidelity achievable is increasing continuously; one benefit of MCNPX is that it allows us to look at fine-tuned 2-D response.

Burnup Accumulation per Location for 4 wt% Case in Library #2

Step #	Time Step (d)	Position 1	Position 2	Cumulative	Position 3	Cumulative
1	0.5	0.004	–	26.2	–	44.1
2	4	0.3	0.2	26.4	0.01	44.1
3	30	2.4	1.7	27.9	0.1	44.2
4	65	6.9	4.8	31.0	0.3	44.4
5	70	11.6	7.9	34.1	0.6	44.7
6	78	16.6	11.3	37.5	1.0	45.1
7	78	21.5	14.7	40.9	1.5	45.6
8	78	26.2	17.9	44.1	2.0	46.1

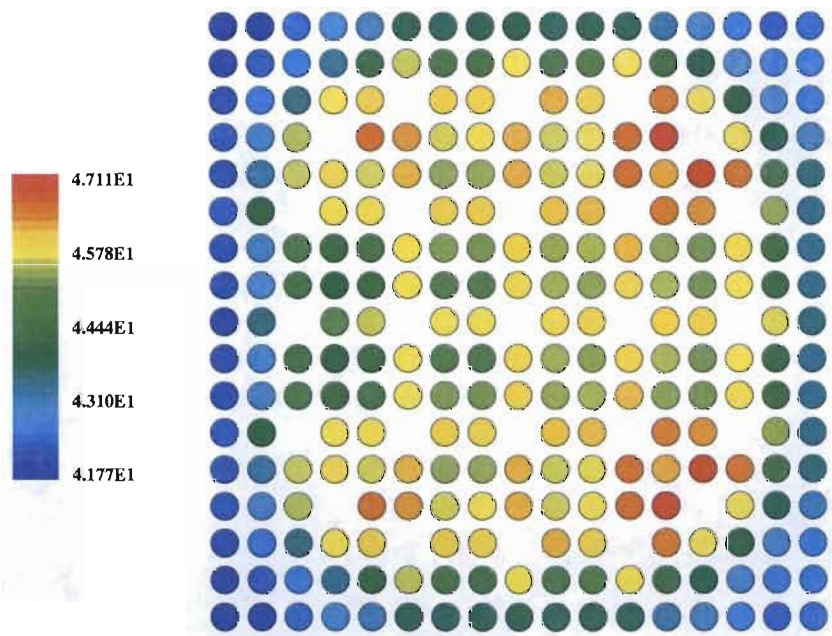
Burnup Comparison of Libraries 1 and 2

MCNP BU4wt45GWd.txt



Library #1

Library #2



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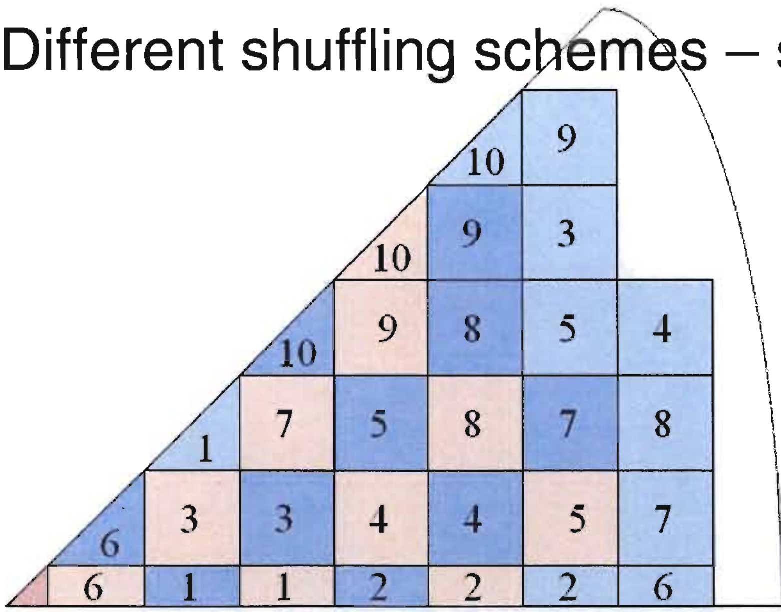
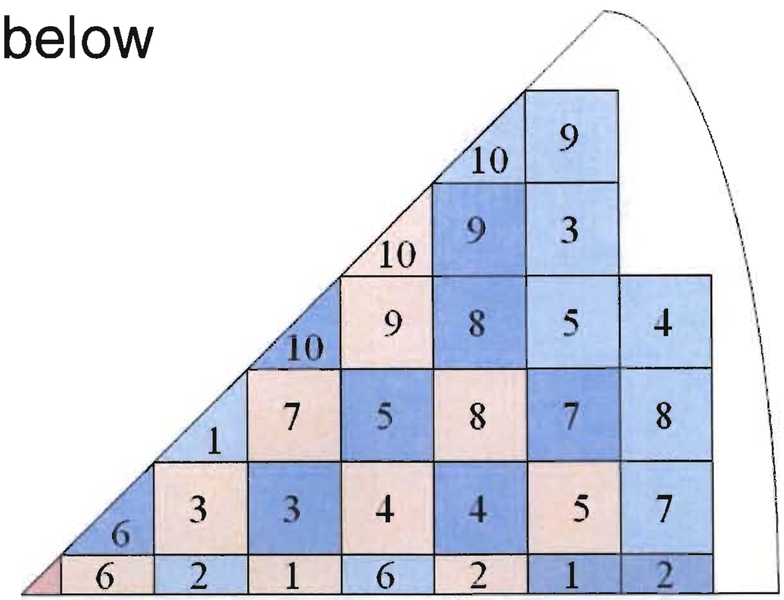
Further Calculations

- Sensitivity studies with 4wt% IE
- Variations in water/fuel temperature
- Presence/absence of control rods/burnable poisons
- Different shuffling schemes – see below

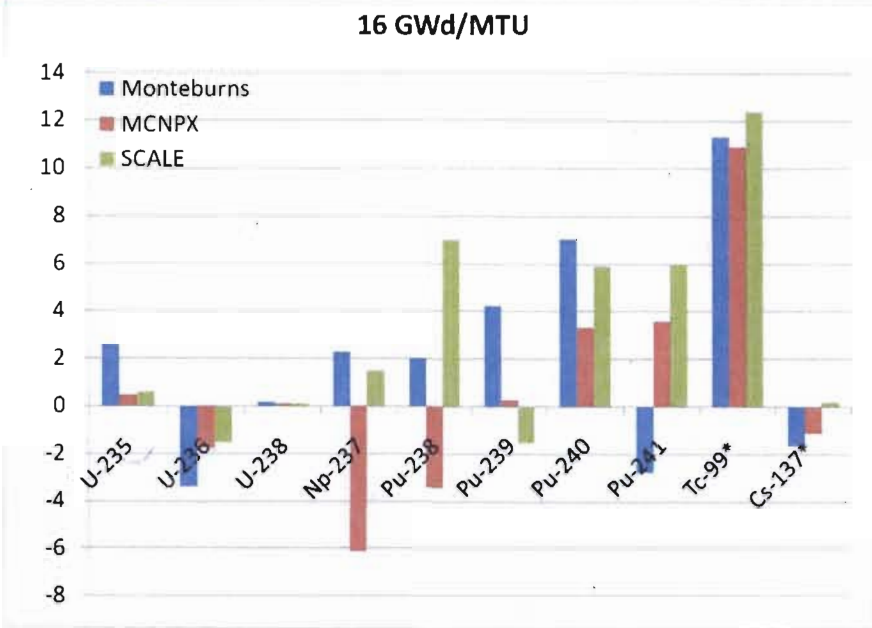


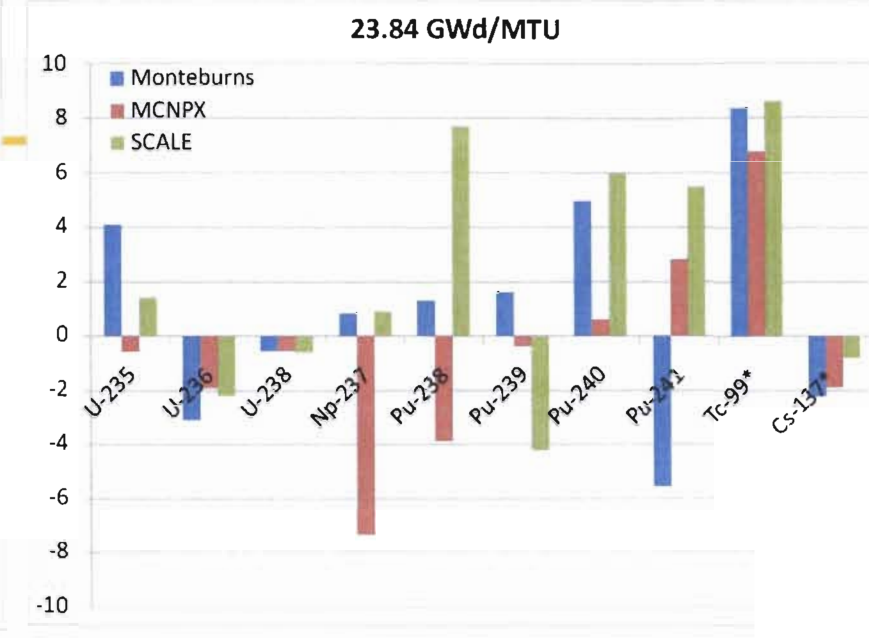
Shuffling Scheme 2

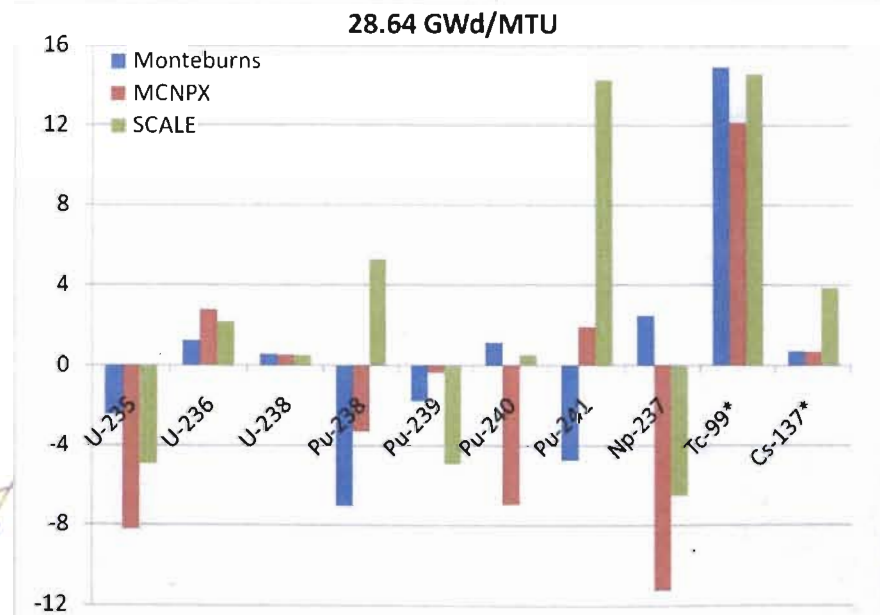


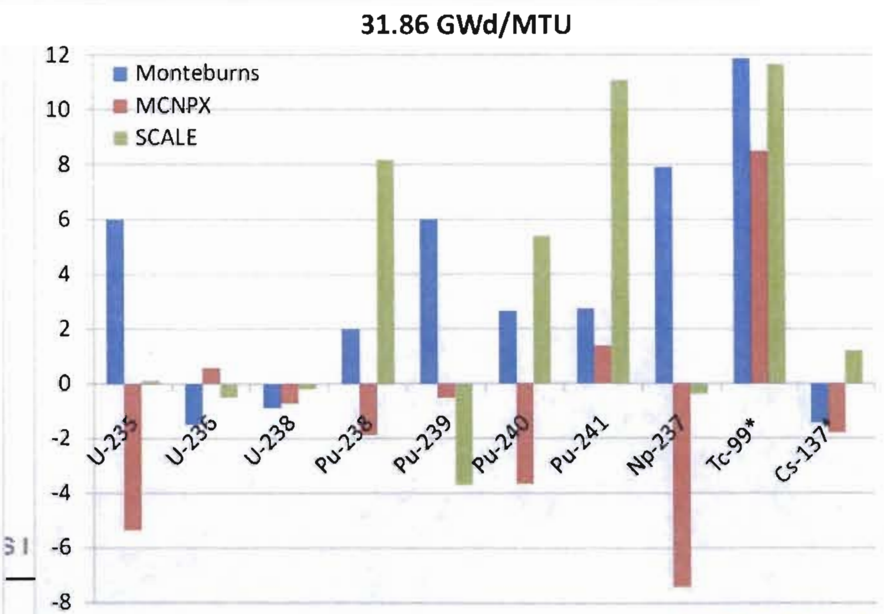
Shuffling Scheme 3 – Older Pattern

Relative Percent Error Code Comparisor

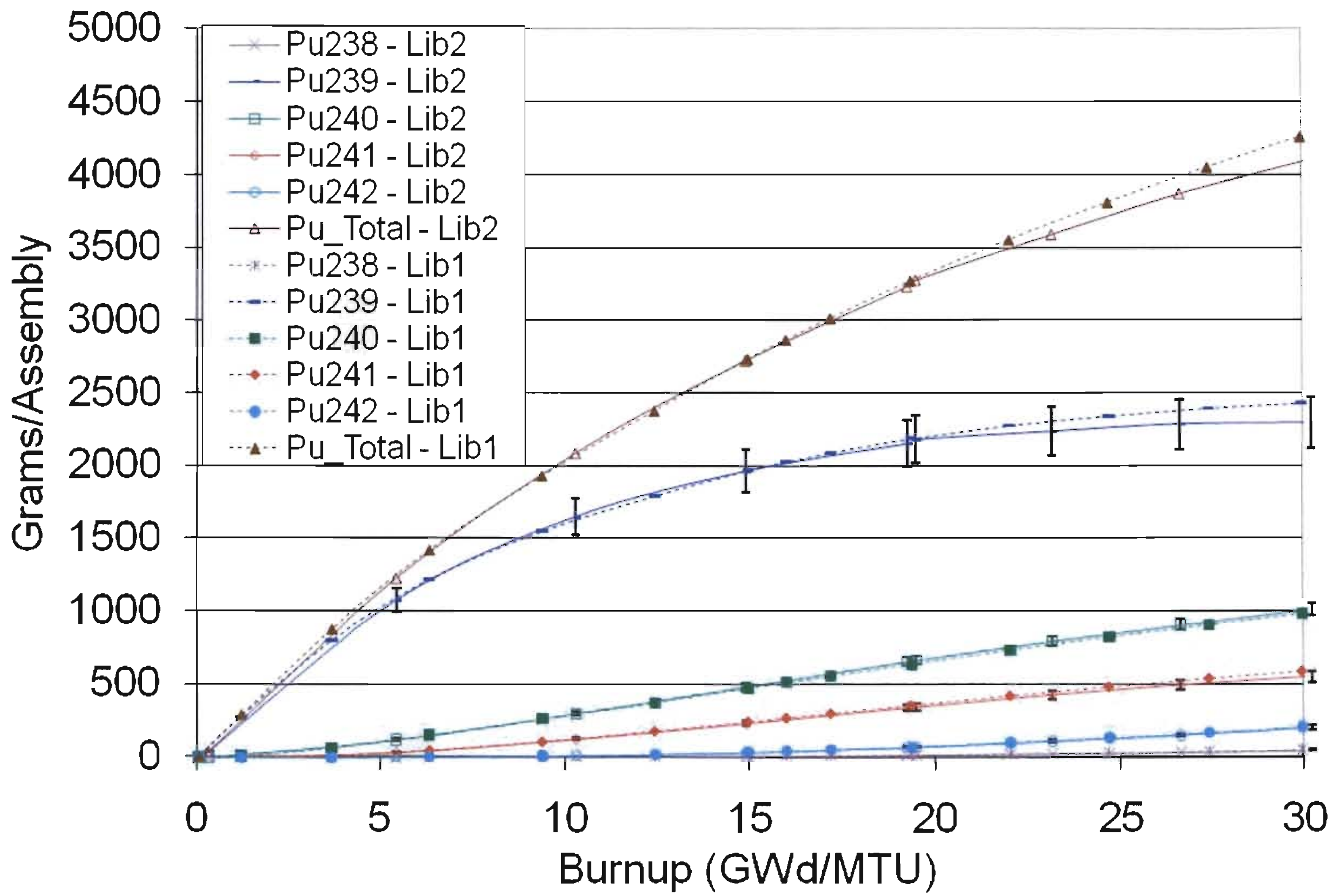




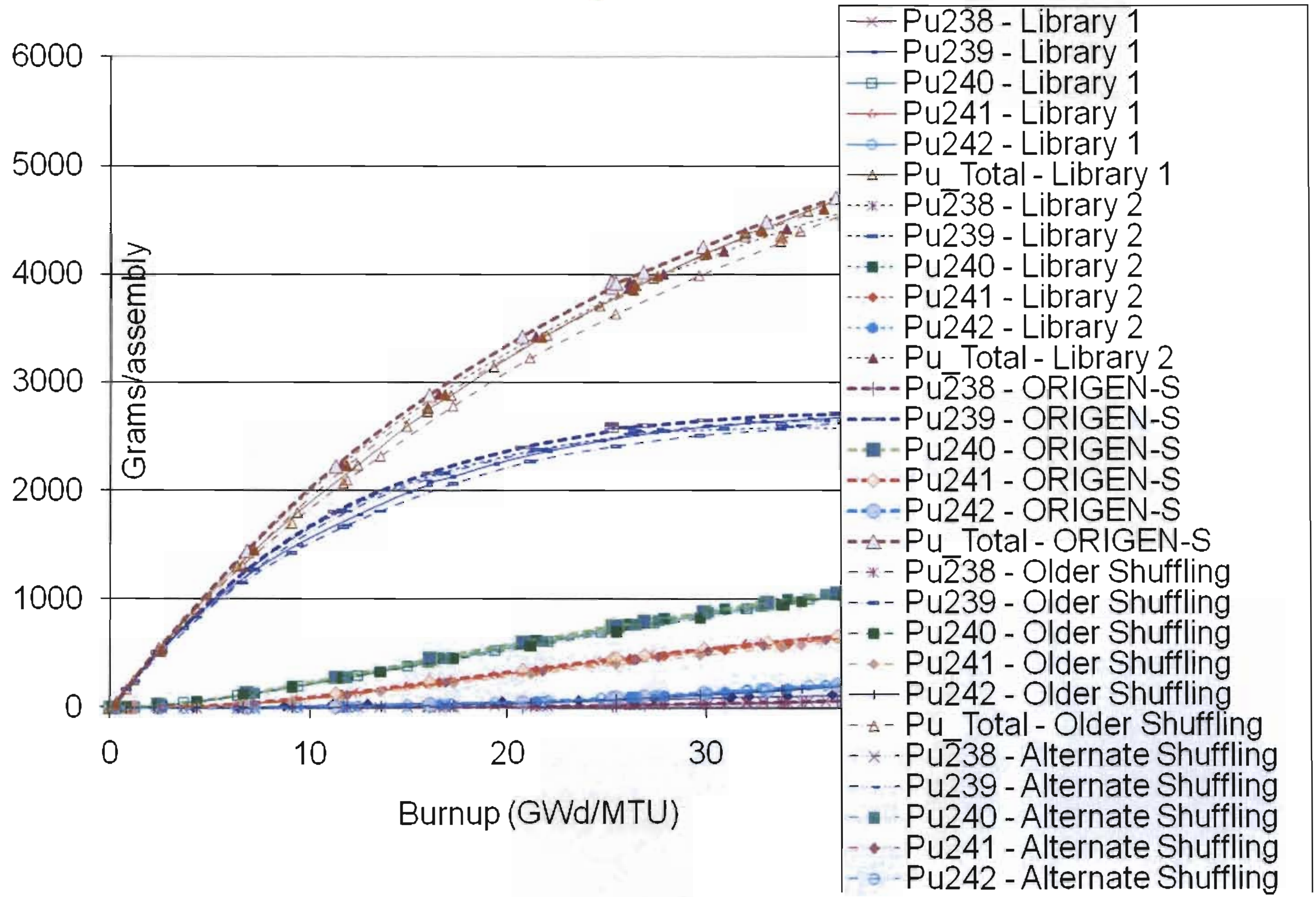




Plutonium Isotopic Correlations for 3wt%



Plutonium Isotopic Correlations for 4wt%



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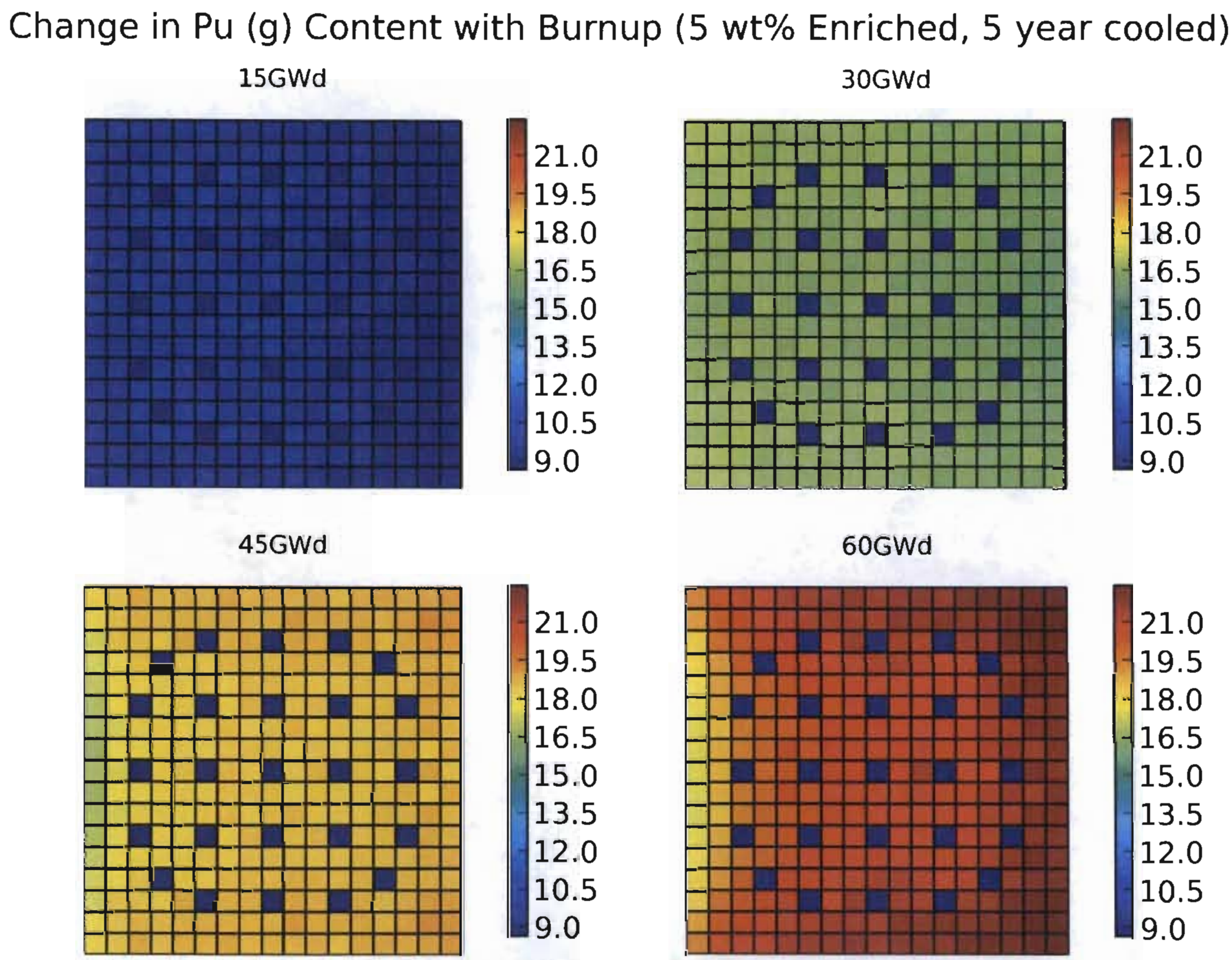
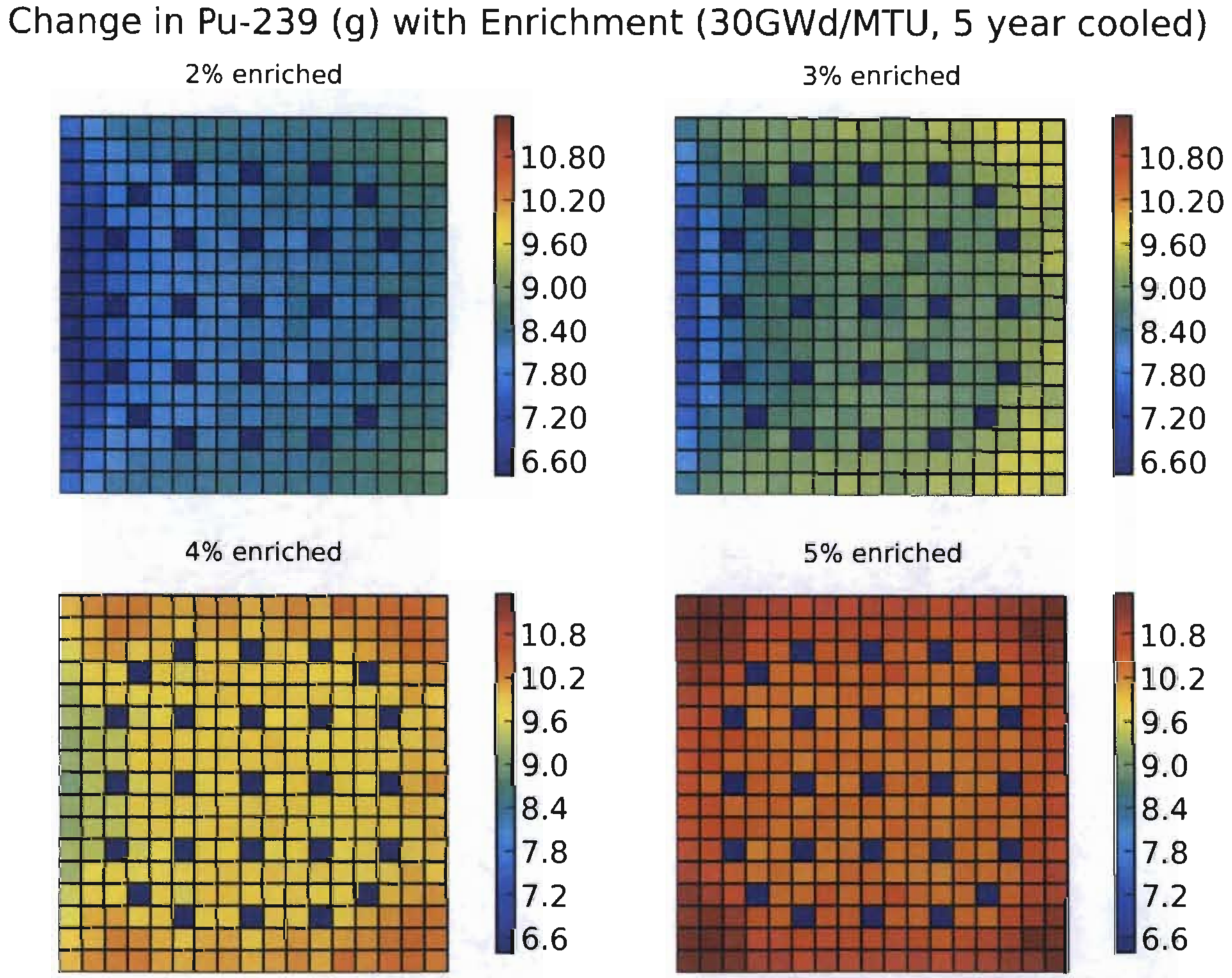
Change in Pu Content With Burnup

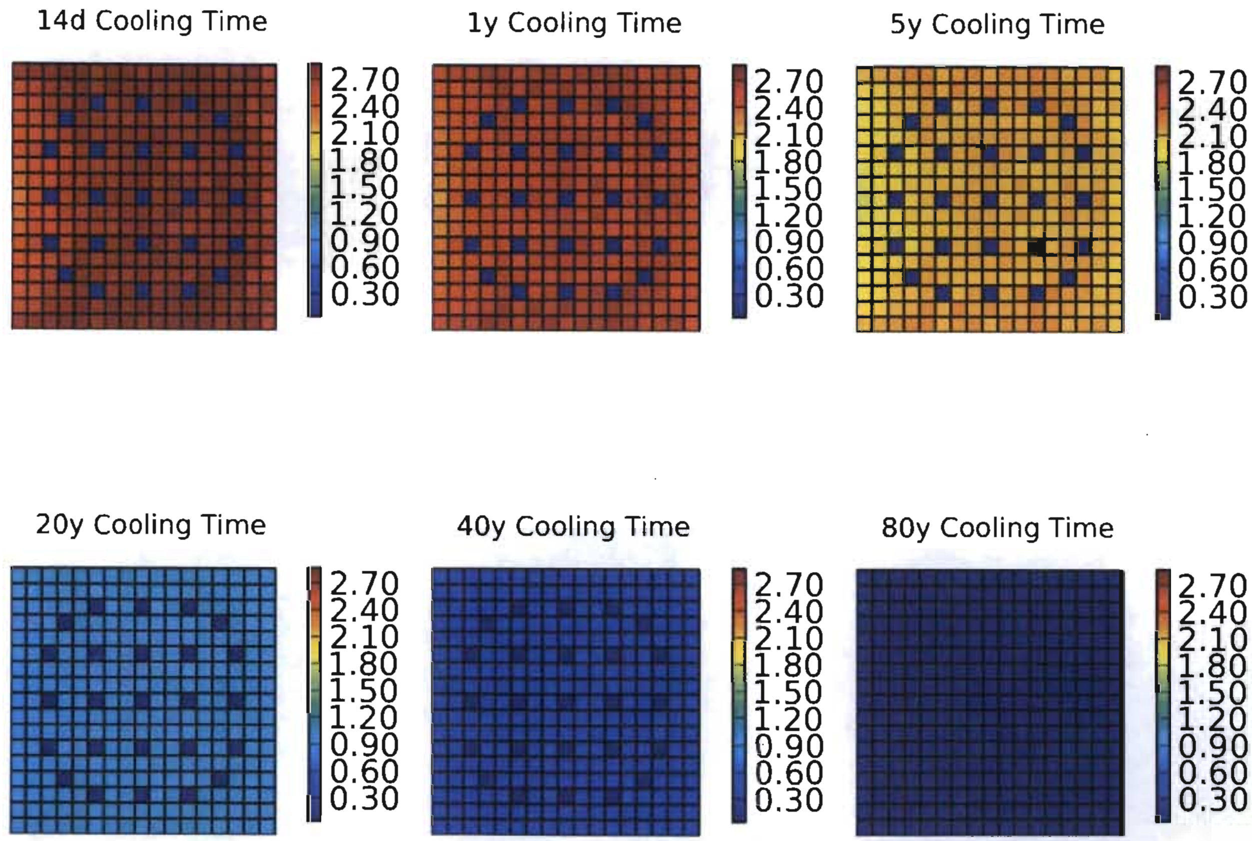


Change in ^{239}Pu with Enrichment

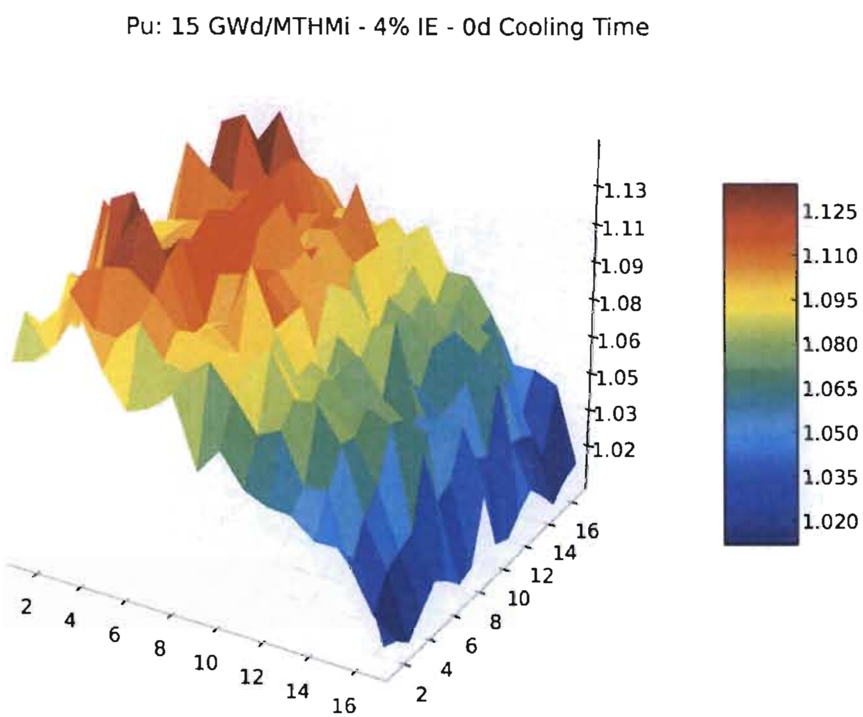


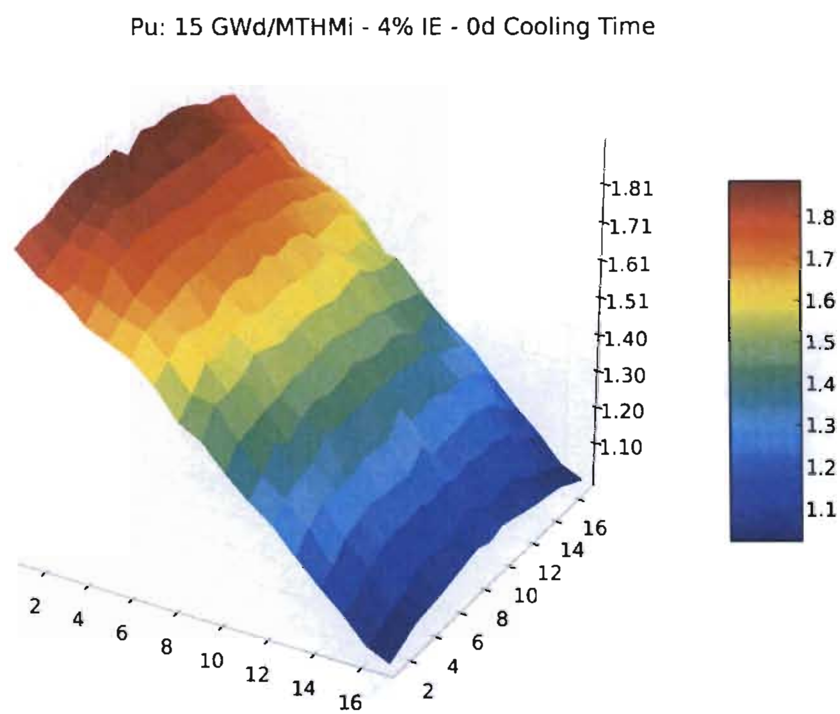
Change in ^{241}Pu with Cooling Time

Change in Pu-241 (g) with Cooling Time (45 GWd/MTU, 4 wt% Enriched)

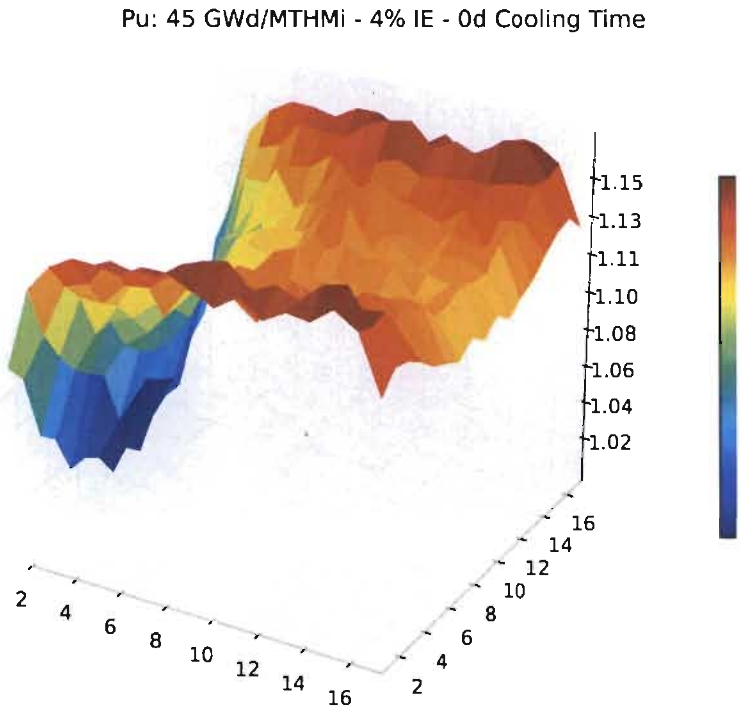


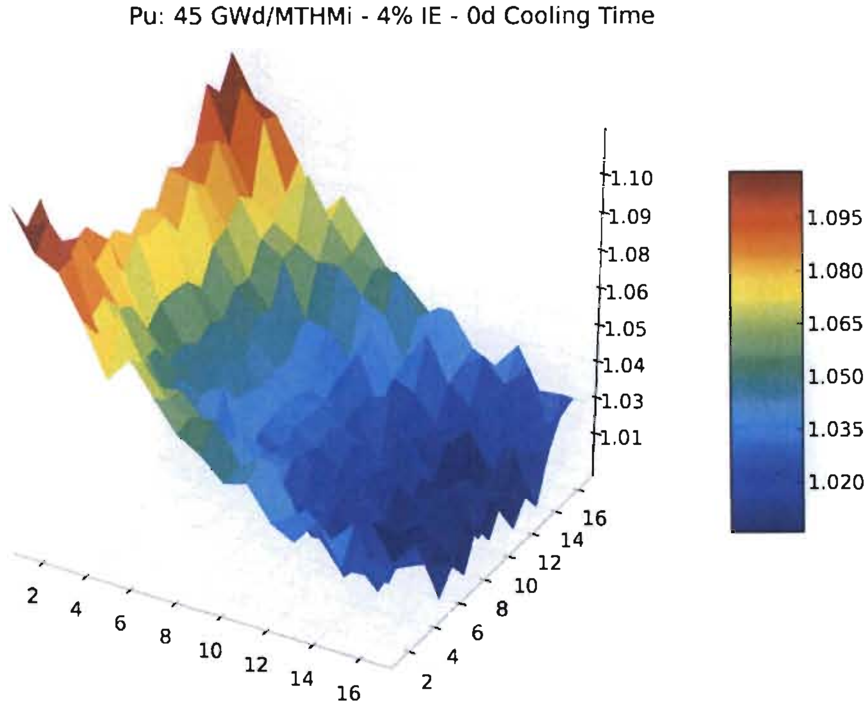
Distribution of Pu for Various Shuffling Schemes – low BU





Distribution of Pu for Various Shuffling Schemes – high BU





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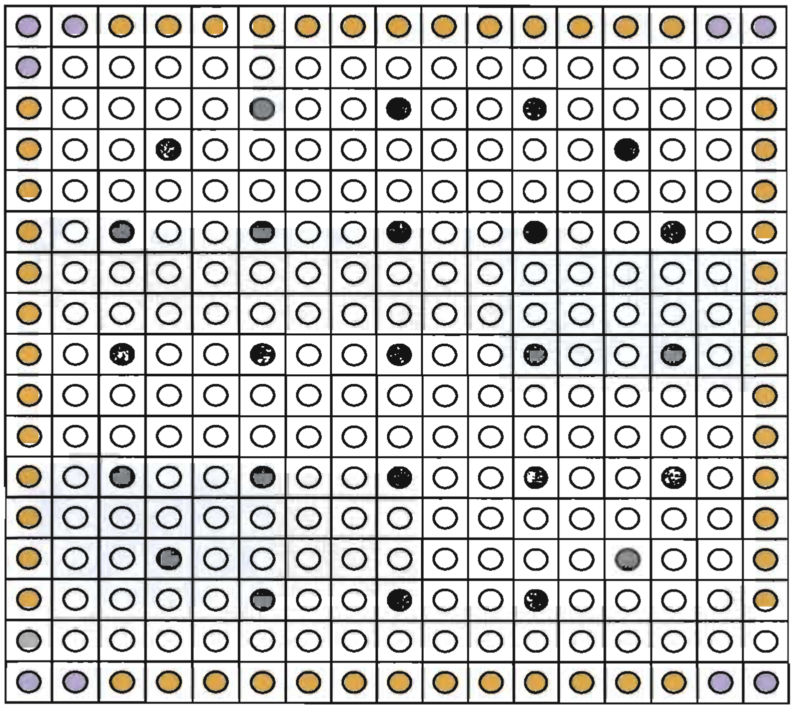
Conclusions/Future Work

- The first library yields valuable information about the effect of burnup, initial enrichment, and cooling time on various detectors.
- The second and future libraries give information for sensitivity studies and potential assembly outlyers.
- Monte Carlo burnup calculations have been benchmarked for low BU, low IE conditions and perform adequately.
- The authors would like to acknowledge the support of the Next Generation Safeguards Initiative (NGSI), Office of Nonproliferation and International Security (NIS), National Nuclear Security Administration (NNSA).

Additional Slides

Position of Control/Shutdown Rods and Burnable Poisons



○ = Fuel Rod

● = Wet Annular Burnable Absorber Or Guide Tube

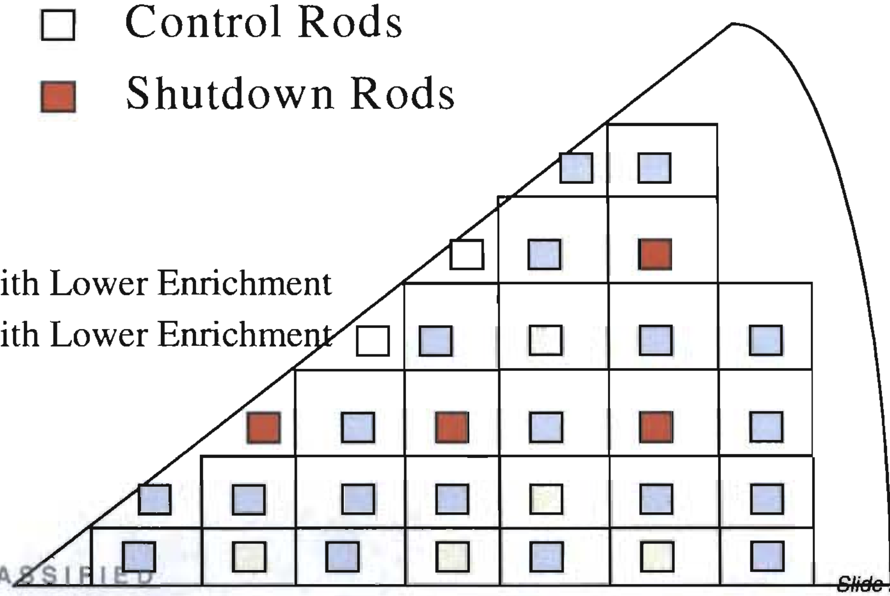
○ = Fuel Rod with Lower Enrichment

● = Fuel Rod with Lower Enrichment

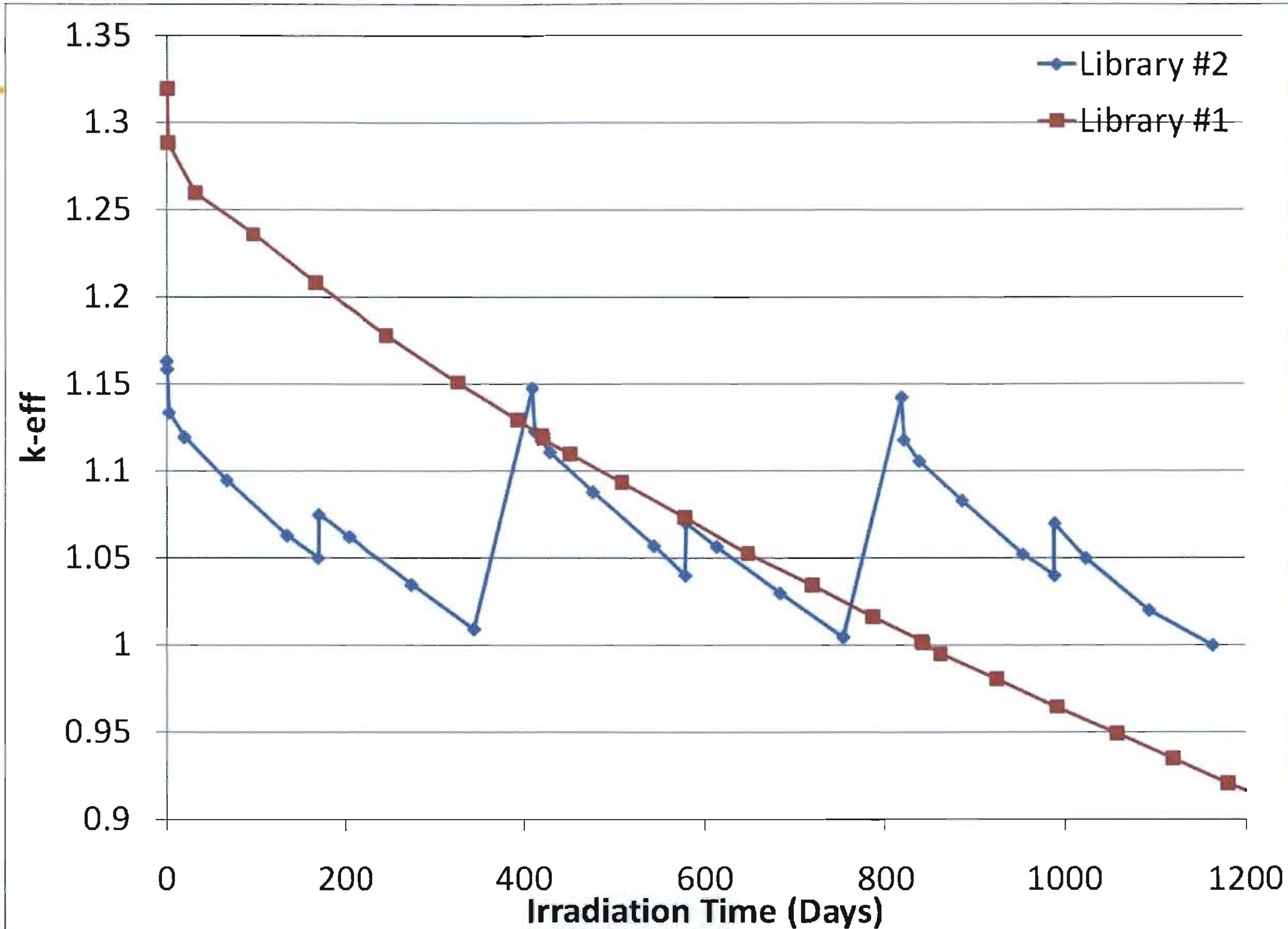
□ No Shutdown/Control Rods

□ Control Rods

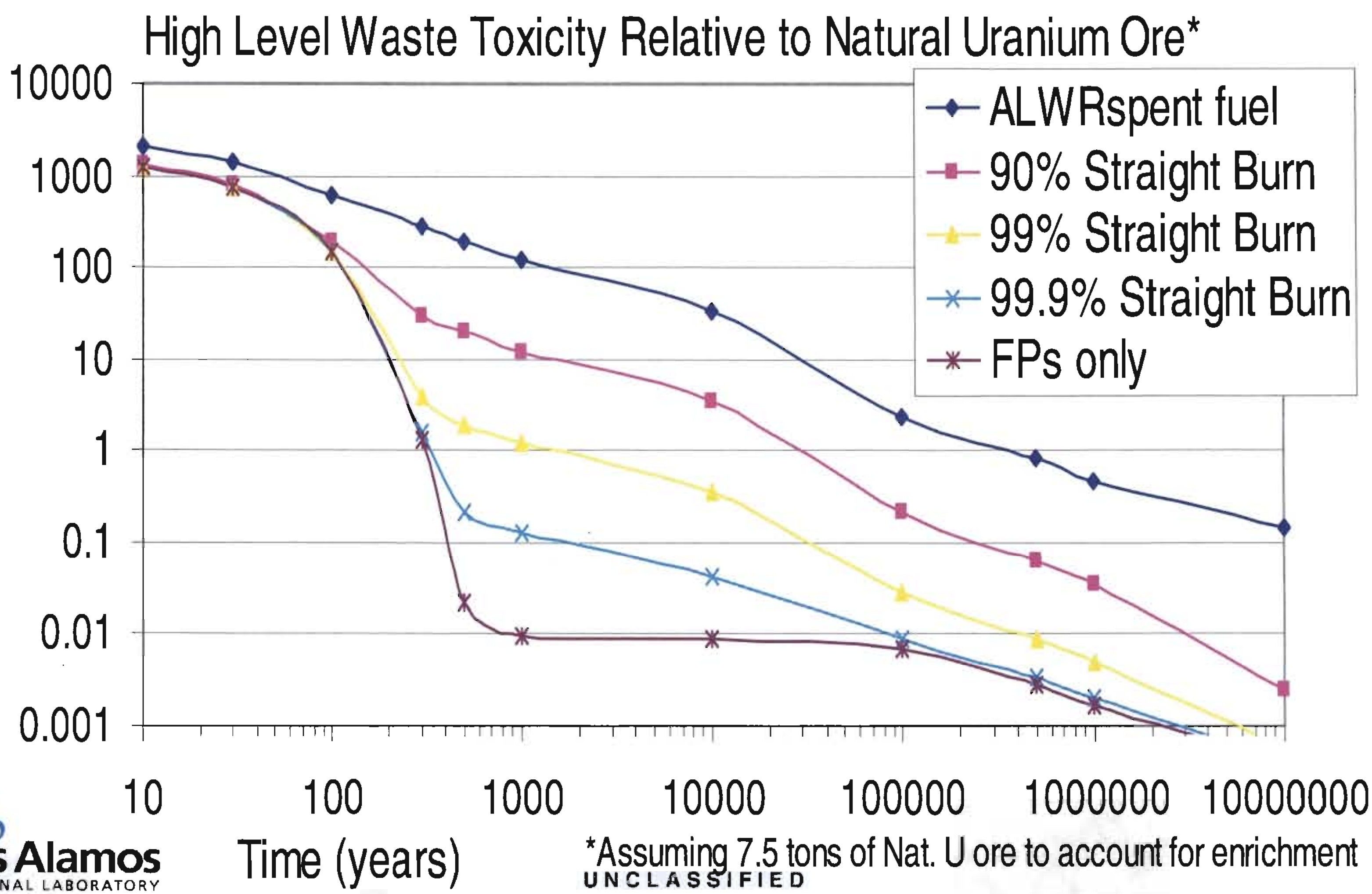
■ Shutdown Rods



Reactivity as a Function of Case

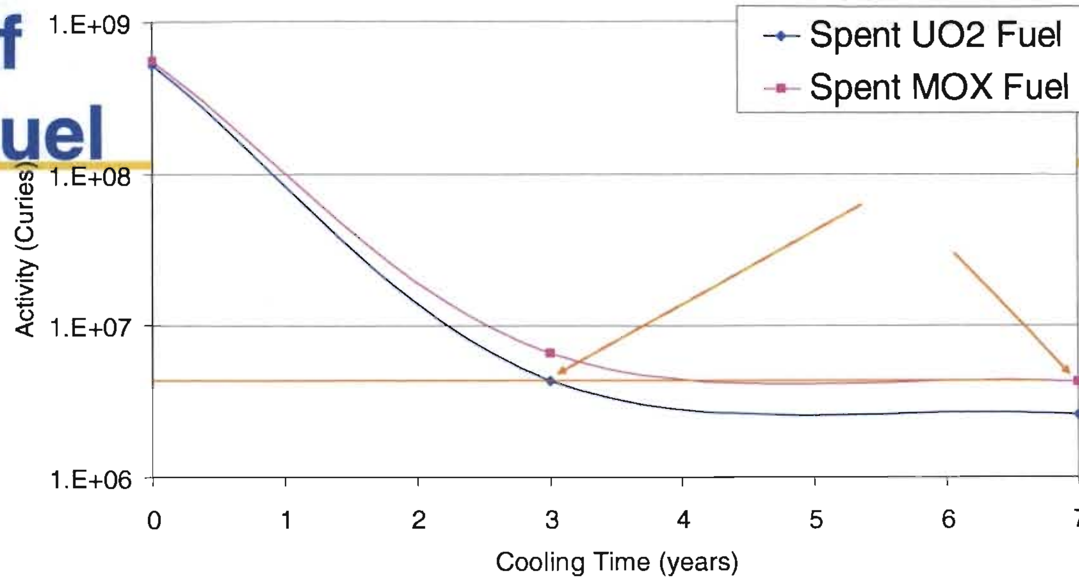


Radiotoxicity of Spent Fuel

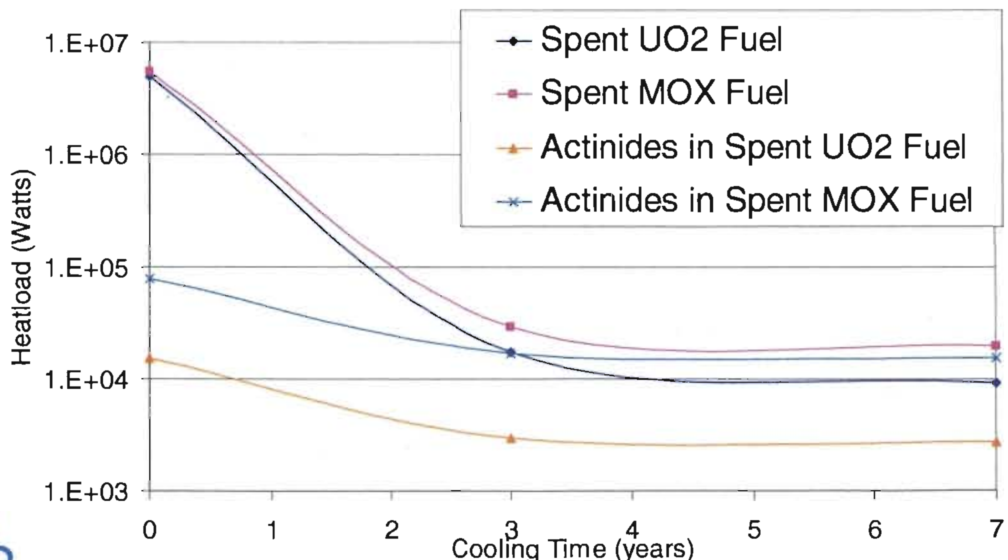


*Assuming 7.5 tons of Nat. U ore to account for enrichment

Activity and Heatload of Spent MOX Fuel



Activity of spent UO2 fuel after 3 years is equal to that of spent MOX fuel after 7 years



Heatload of spent UO2 fuel after 3 years Is equal to that of spent MOX fuel after 7 years

Pin Cell Benchmark 3.2% ^{235}U, 27.35 GWd/MTU

*M. D. DEHART, M. C. BRADY, and C. V. PARKS, "OECD/NEA Burnup Credit Calculational Criticality Benchmark Phase I-B Results," NEA/NSC/DOC(96)-06 and ORNL-6901, Oak Ridge National Laboratory (June 1996).

Isotope	Published (mg/g UO_2)	*Monteburns* (mg/g UO_2)	MCNPX (mg/g UO_2)	% Error	2 % Error	Range from Other Codes
U-234	0.160	0.156	0.142	-2.45	-11.1	0.133 to 0.175
U-235	8.47	8.10	8.34	-4.32	-1.54	7.44 to 8.66
U-236	3.14	3.21	3.17	2.09	1.06	3.128 to 3.540
U-238	843	838	838	-0.50	-0.59	836.7 to 841.5
Np-237	0.268	0.286	0.279	6.65	4.25	0.253 to 0.340
Pu-238	0.101	0.095	0.094	-6.12	-6.67	0.0572to 0.108
Pu-239	4.26	3.94	3.89	-7.50	-8.74	3.660 to 4.690
Pu-240	1.72	1.68	1.64	-2.00	-4.60	1.573 to 1.860
Pu-241	0.681	0.663	0.662	-2.72	-2.90	0.531 to 0.734
Pu-242	0.289	0.308	0.307	6.65	6.36	0.200 to 0.319