LA-UR- 11-01879

Approved for public release;
distribution is unlimited.

Title: Description of the Spent Nuclear Fuel Library

Author(s): Holly R. Trellue
Michael L. Fensin
Jack D. Galloway

Intended for: NGSI Review Committee
Los Alamos, NM April 4, 2011

Los Alamos
NATIONAL LABORATORY
EST. 1943

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.

Description of the Spent Nuclear Fuel Library

Holly R. Trellue

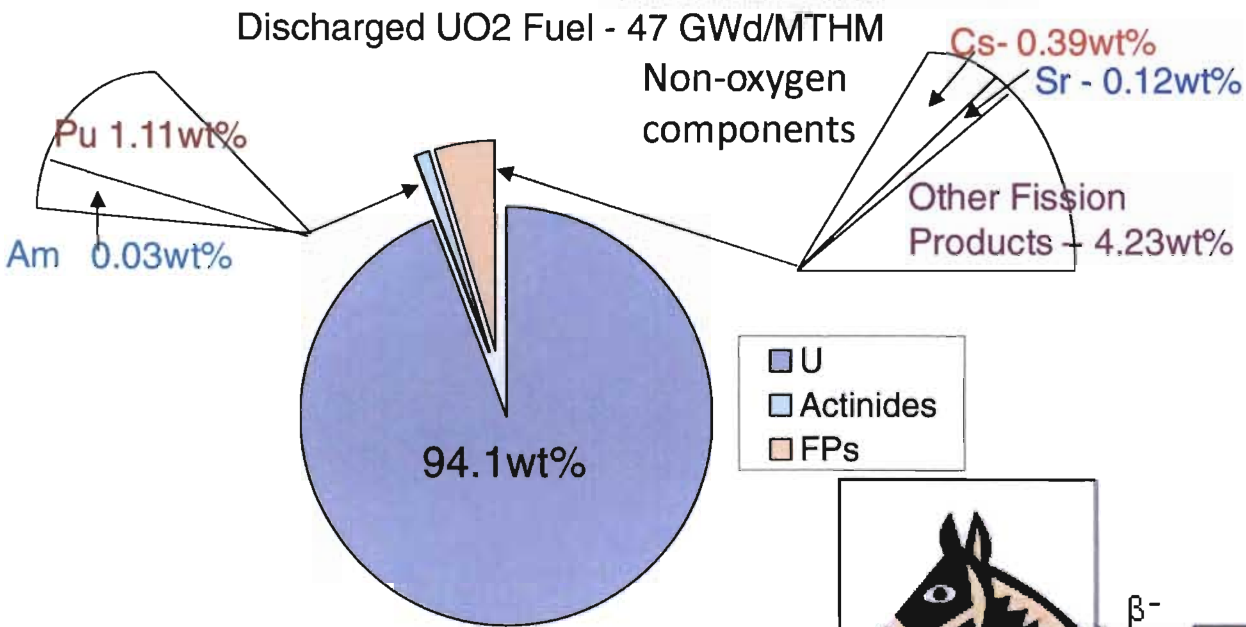
Michael L. Fensin

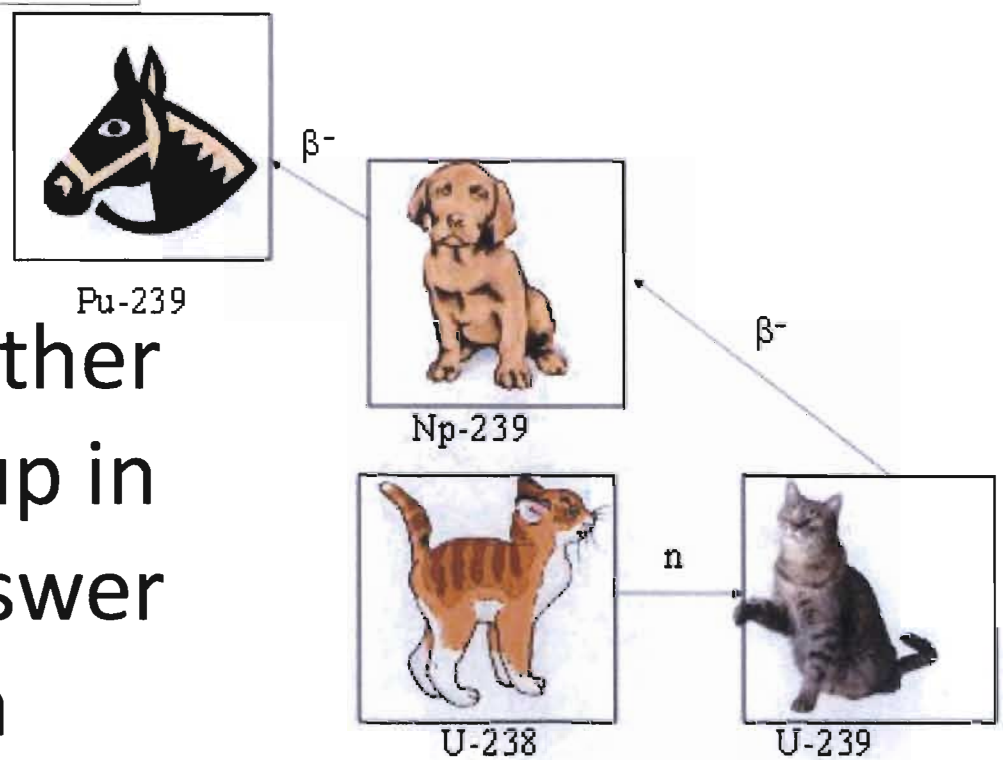
Jack D. Galloway

Los Alamos National Laboratory, D-5

trellue@lanl.gov

Used Fuel Composition



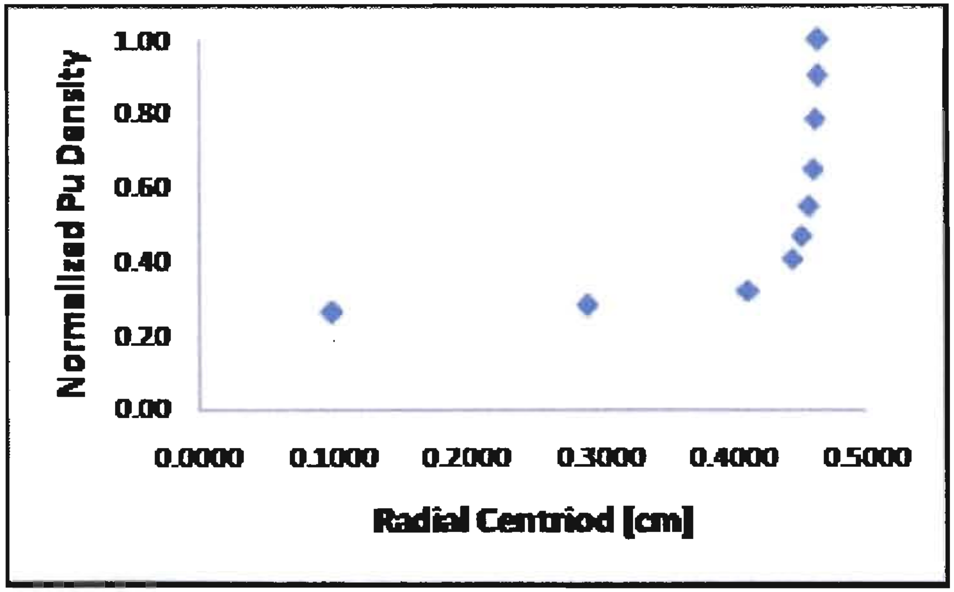


How Do Materials Other Than Uranium End up in Spent Fuel? The Answer is Transmutation

Introduction

- To limit scope of the NGSI project, only Pressurized Water Reactor (PWR) used fuel assemblies are modeled; not Boiling Water Reactor (BWR) ones.
- A total of three spent fuel libraries have been/will be developed with various burnups (BU).

1. Infinitely-reflected assembly calculations the first year with 4 radial fuel regions with as much fidelity as possible at the time. (Mike Fensin)
2. "Representative" shuffled assembly tracked through PWR shuffling scheme last Fall with 1 radial region. (Holly Trellue)
3. Sensitivity study on various parameters for 4wt% initial enrichment (IE): shuffling, temperature, addition of control rods/burnable poison in assembly, etc. (Holly Trellue, Matthew Francis - ORNL)

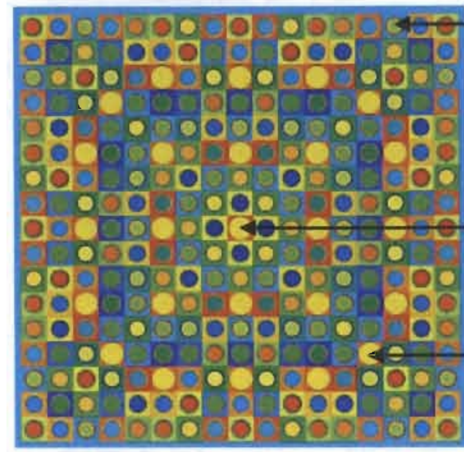


Case Description

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



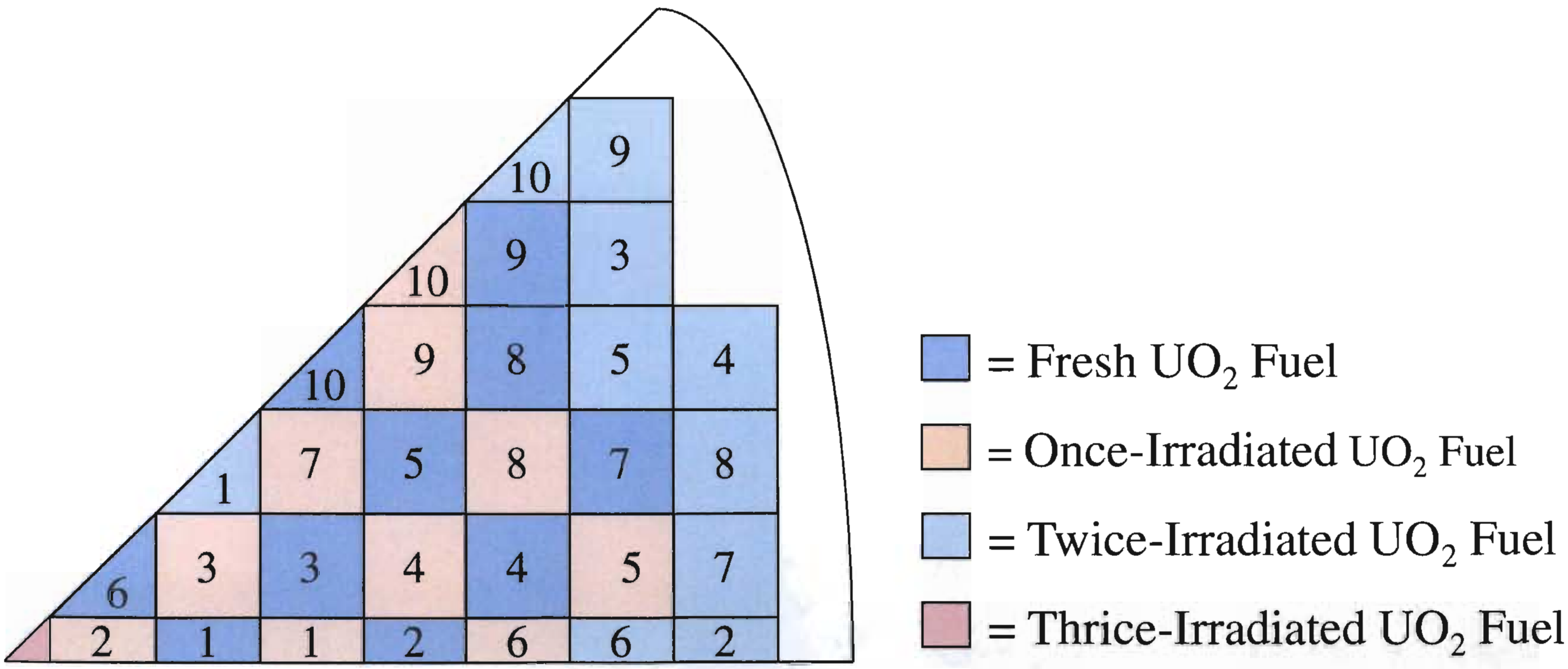
- Infinitely-reflected generic 17 X 17 PWR; 39 rods symmetrically modeled in 1/8 of an assembly.
  - UO_2 fuel; Zircaloy-4 clad; no gap
  - Axially homogenous
- Dimensions obtained from OECD/NEA IVB Benchmark
- Radial zones per pin: 0.39, 0.402, 0.4075, and 0.41 cm.
- ~2 GWD/MTU time durations after Xe and Sm equilibrium
- 1 and 4 weeks, 1, 2, 5, 20, 80 year cooling times
- 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* (Limited Isotope Inclusion)
- Fuel and Fuel Cross sections were for a temperature of 900 K
- Average boron concentration in water was 660 ppm; 575 K Water Temp.
- 600 K Cladding and Water Cross Sections were used.

Library #2

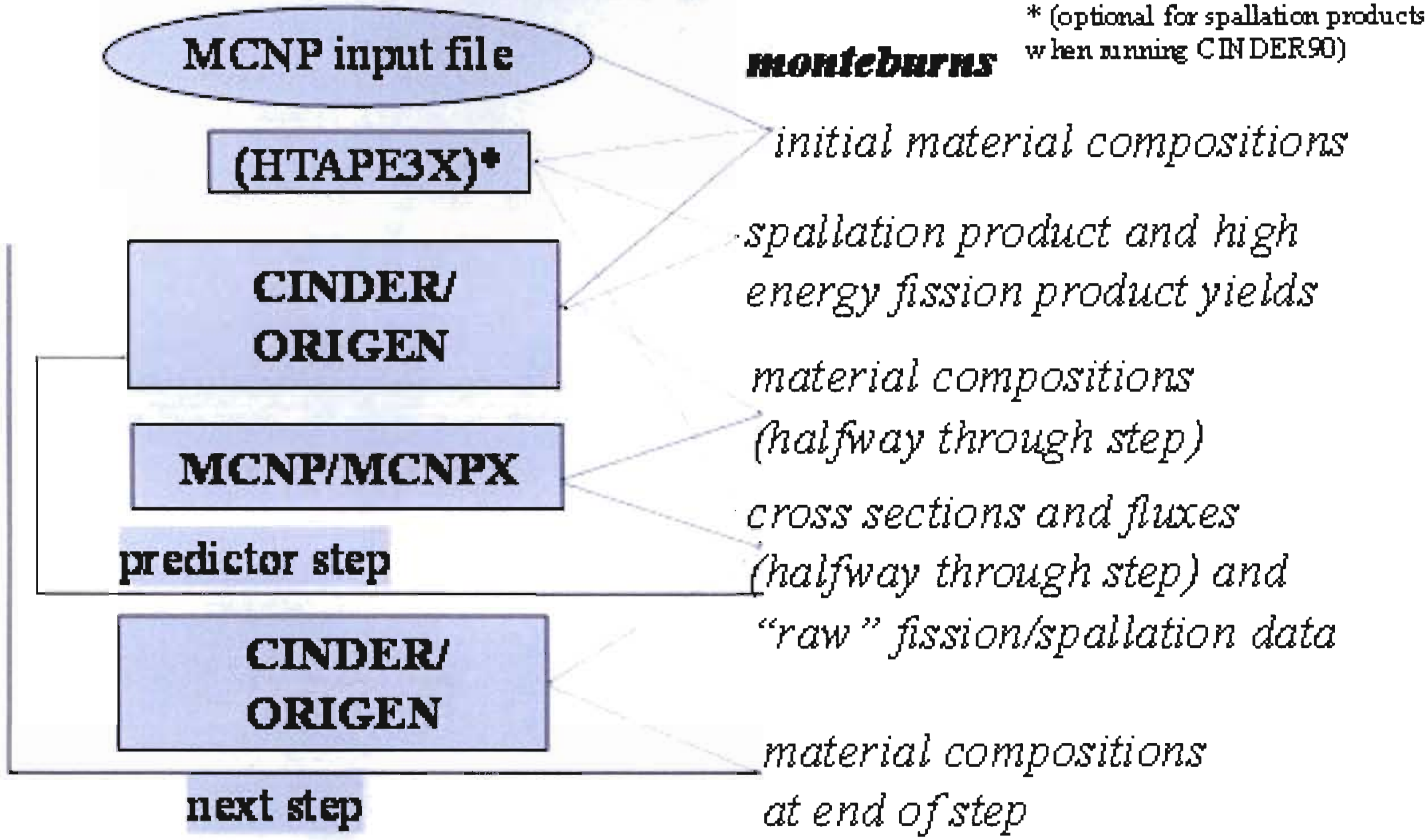
- Asymmetric burn of assembly performed using a 1/8 core reflected core model, 443 burn materials.
- *Monteburns* is used with CINDER90; same premise as MCNPX burnup, just different linkage tool.
- Includes ^{234}U enrichment as well as ^{235}U
- Includes 99.9 % of fission product mass (most included as "importance fraction" in Monteburns: contribution to absorption, fission, mass, or atom fraction)
- Reduced number of IE/BU cases but only 1 radial region.
- CTs of 14 days, 1 yr, 5 yr, 10 yr, 20 yr, and 80 yr
- Length of irradiation time step was tested and same answers were obtained for 40 vs. 80 days, so a longer time steps used.
- 400000 particles/cycle, 100 cycles, 20 skipped cycles, and "accumulating" source files were used.

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, and MCNPX allows us to look at fine-tuned 2-D response.

Isotopes Deemed Important

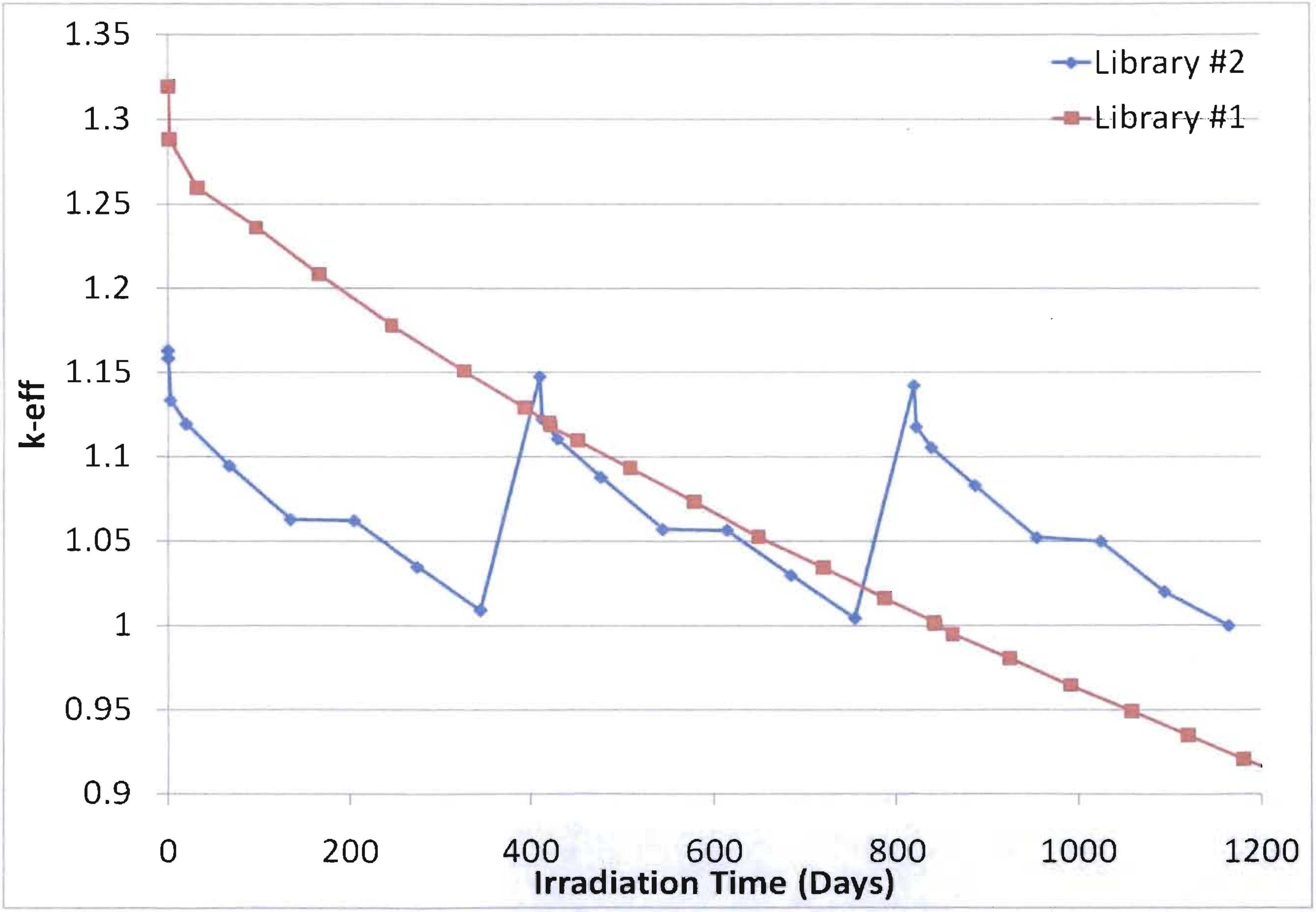
1001	48114	62152	92235
5010	49115	64155	92236
34077	51121	65159	92238
40091	54131	66161	93237
41094	55133	66162	94239
42096	57139	66163	94240
42097	60143	66164	94241
43099	60144	68166	94242
45103	60150	68167	95241
46107	62149	68168	
47107	62151		

= Not Tracked in Tier 2 of MCNPX

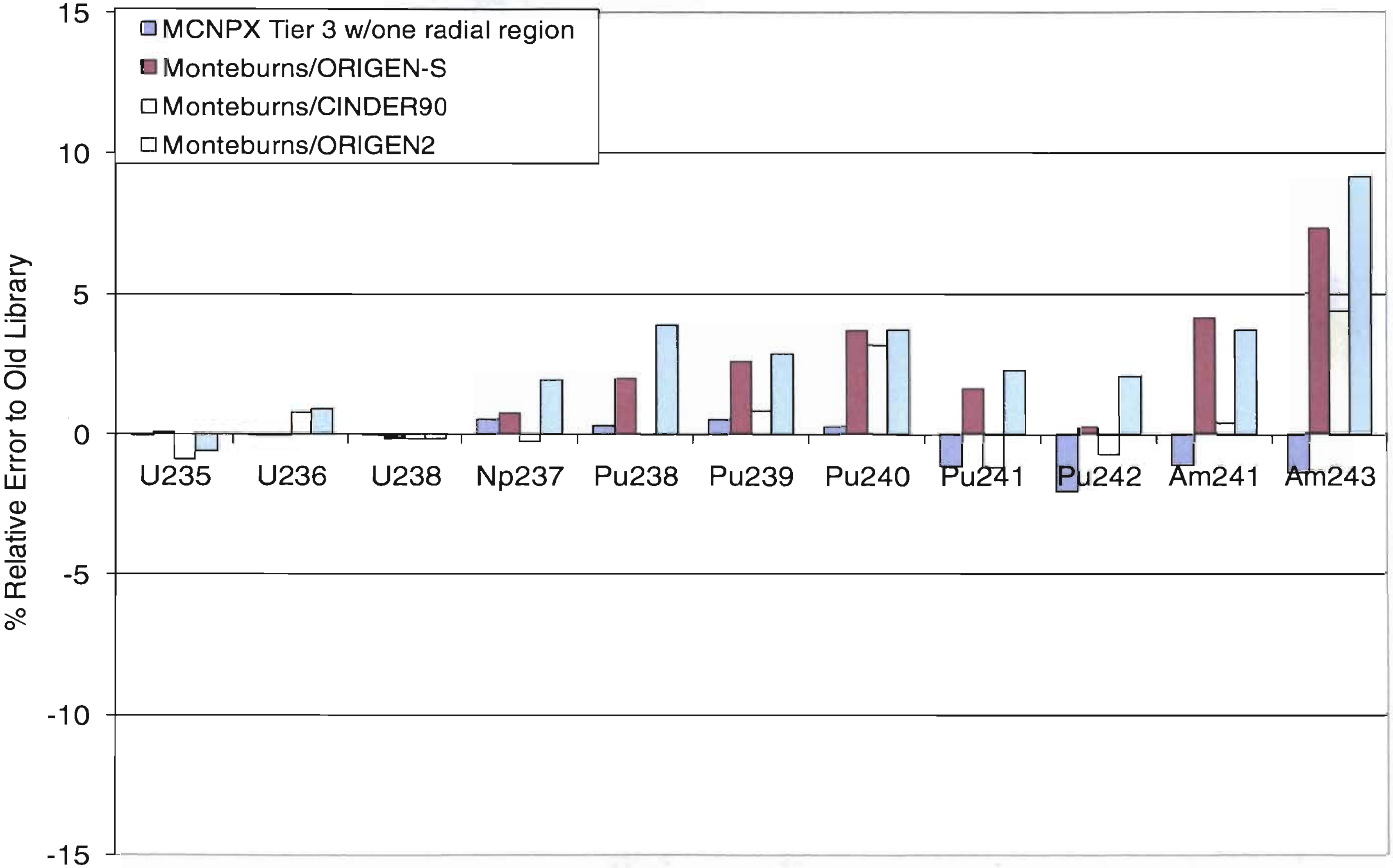
Time Steps for 4 wt% Case in Library #2

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

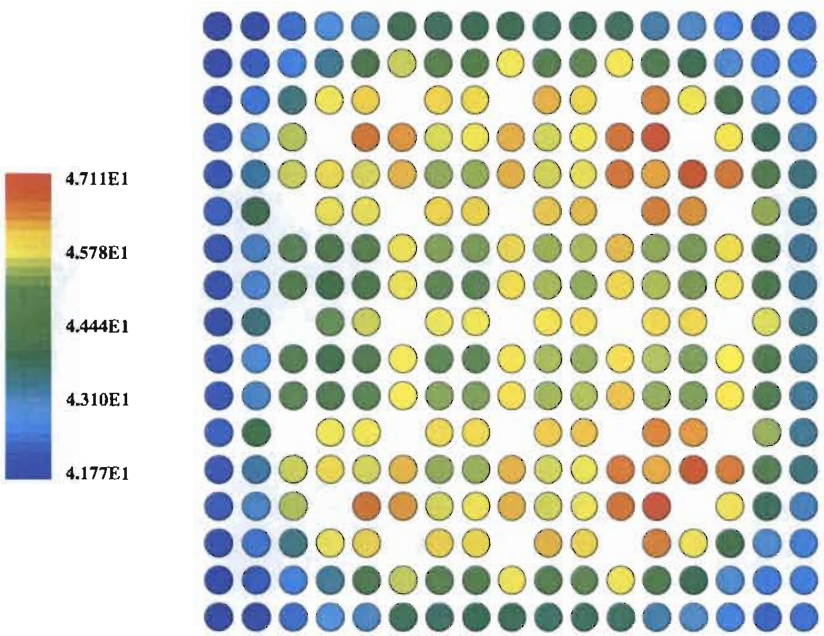
Reactivity as a Function of Case



Code Comparisons



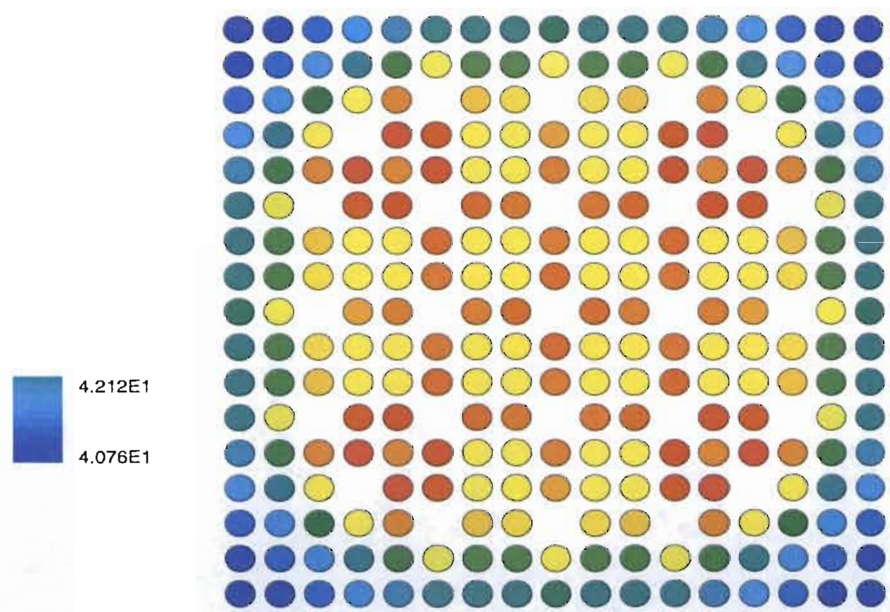
Burnup Comparison of Libraries 1 and 2



Library #2

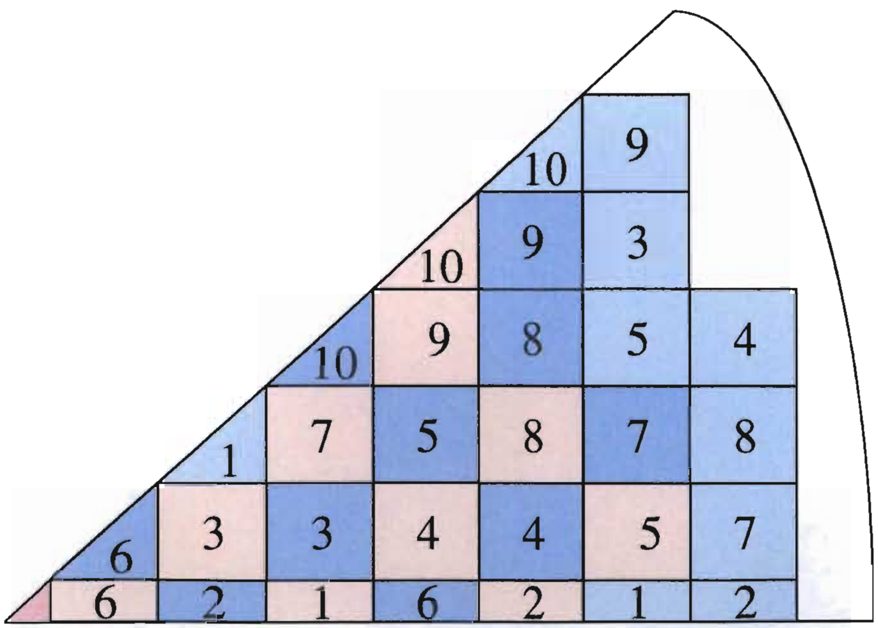
Library #1

MCNP BU4wt45GWd.txt

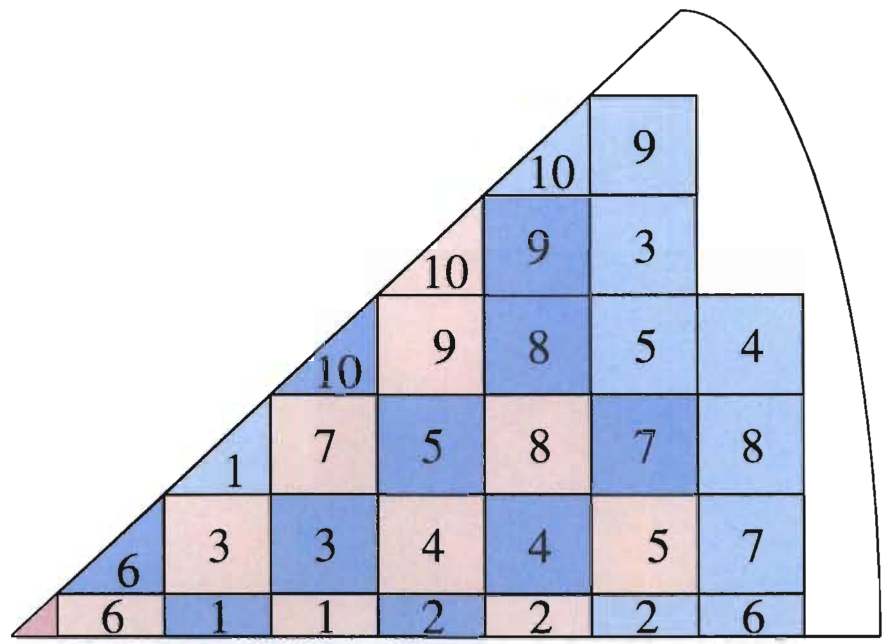


Library #3

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



"Alternate" Shuffling Scheme



"Older" Shuffling Scheme

Benchmark Results for H.B Robinson

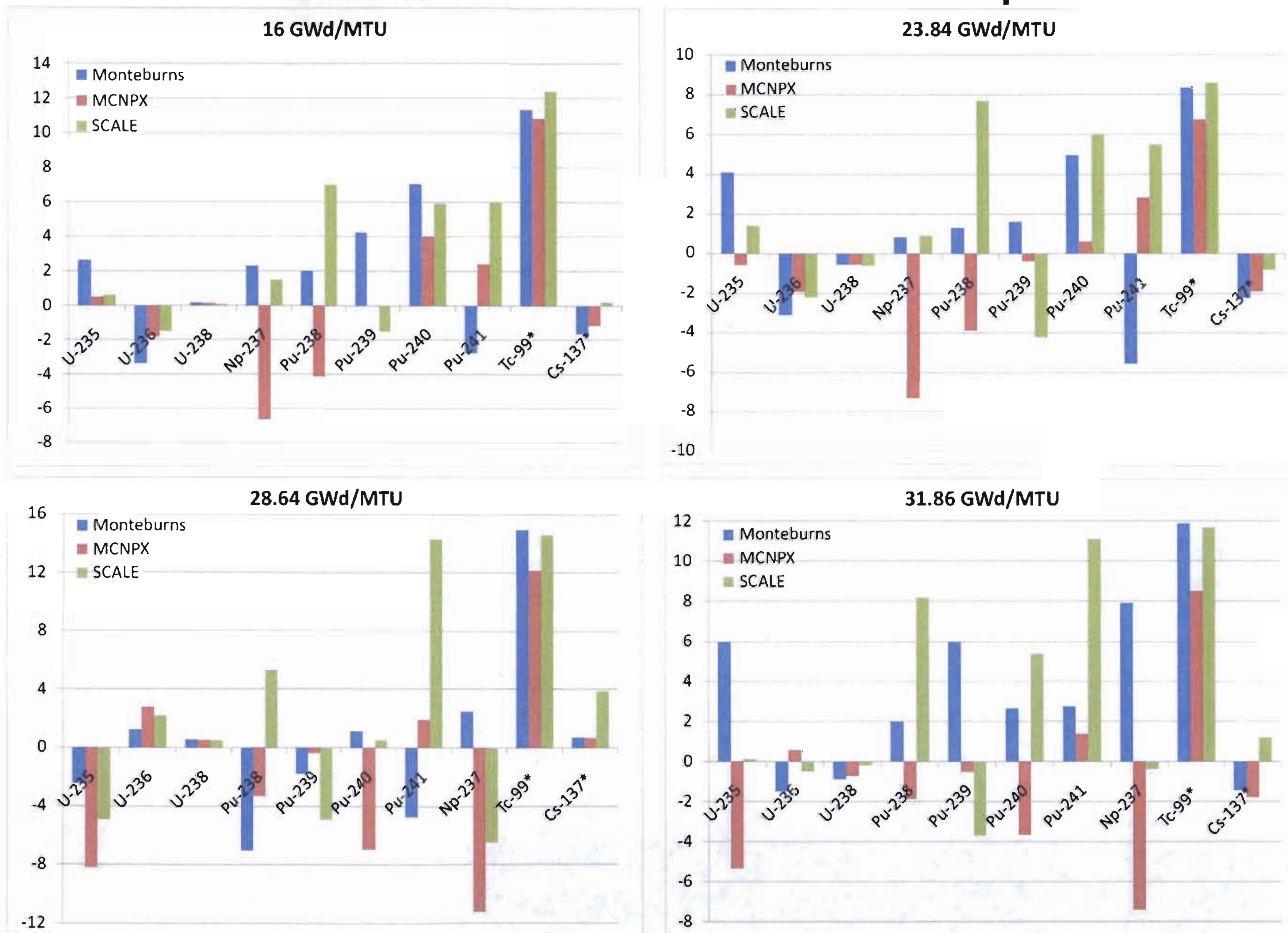
Burnup	16.00 GWd/MTHM			23.84 GWd/MTHM		
Isotope	*monteburns*	published	% error	*monteburns*	published[19]	% error
U-235	0.0110	0.0107	2.62	0.00751	0.00721	4.11
U-236	0.00212	0.00219	-3.37	0.00266	0.00274	-3.09
U-238	0.848	0.847	0.17	0.842	0.847	-0.53
Pu-238	2.89E-05	2.83E-05	2.29	7.01E-05	6.95E-05	0.83
Pu-239	0.00371	0.00364	2.01	0.00407	0.00402	1.31
Pu-240	0.00114	0.00109	4.22	0.00170	0.00167	1.61
Pu-241	3.25E-04	3.04E-04	7.04	5.29E-04	5.04E-04	4.97
Np-237	1.51E-04	1.55E-04	-2.76	2.46E-04	2.60E-04	-5.55
Tc-99*	6.06E-06	5.44E-06	11.35	8.76E-06	8.09E-06	8.34
Cs-137*	0.0353	0.0359	-1.64	0.0527	0.0539	-2.22

Benchmark Results (Cont.)

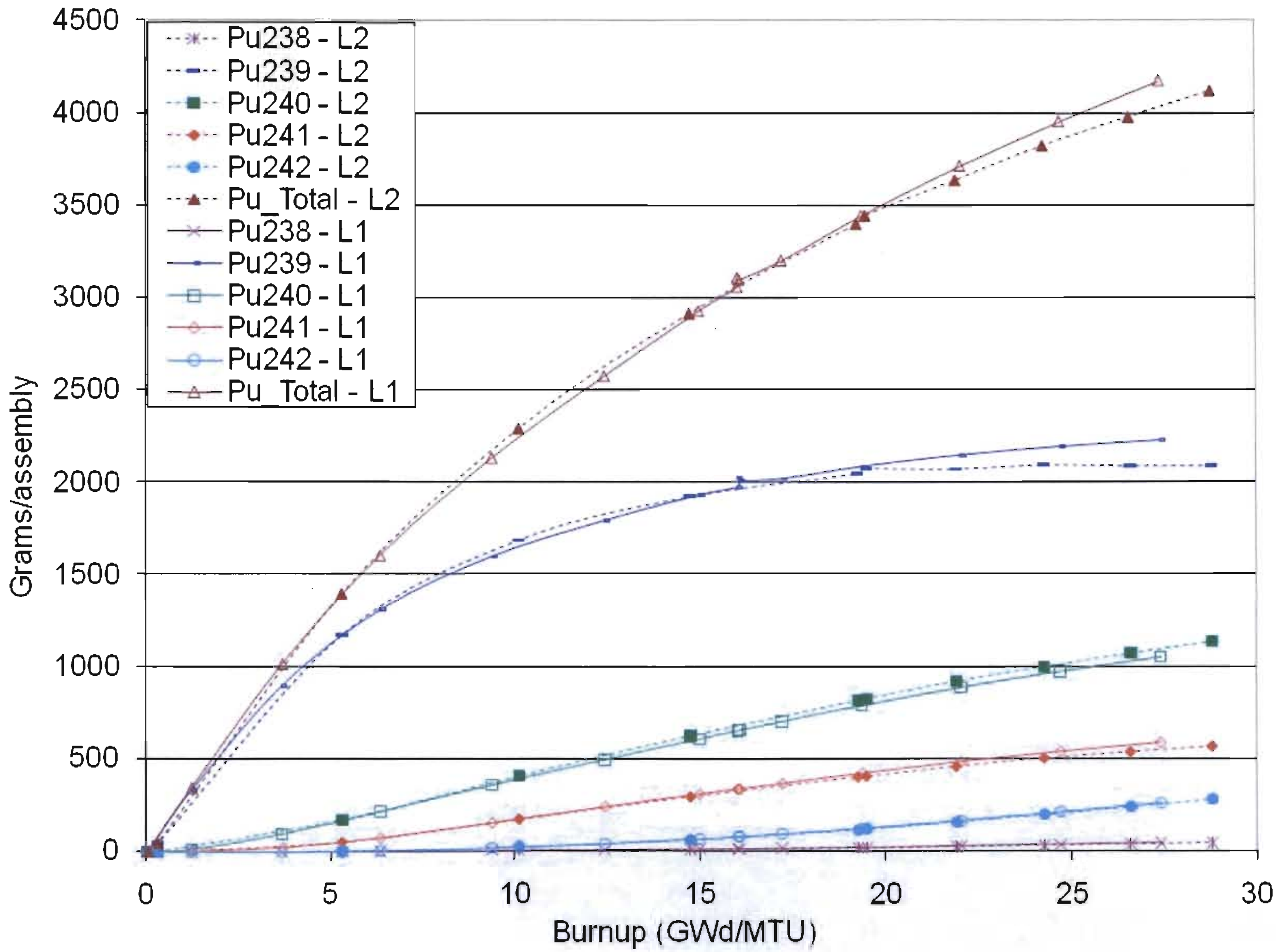
Burnup	**28.64 GWd/MTHM**			**31.86 GWd/MTHM**		
Isotope	*monteburns*	published	% error	*monteburns*	published	% error
U-235	0.00603	0.00618	-2.44	0.00515	0.00486	5.98
U-236	0.00285	0.00282	1.24	0.00295	0.00300	-1.51
U-238	0.838	0.834	0.54	0.835	0.842	-0.89
Pu-238	1.06E-04	1.14E-04	-7.01	1.33E-04	1.30E-04	1.97
Pu-239	0.00431	0.00439	-1.77	0.00445	0.00420	6.00
Pu-240	0.00199	0.00197	1.14	0.00218	0.00212	2.65
Pu-241	6.49E-04	6.81E-04	-4.72	7.11E-04	6.92E-04	2.71
Np-237	3.11E-04	3.04E-04	2.45	3.59E-04	3.33E-04	7.91
Tc-99*	1.03E-05	8.95E-06	14.94	1.13E-05	1.01E-05	11.90
Cs-137*	0.0631	0.0627	0.70	0.0703	0.0713	-1.44

*O. W. HERMANN, S. M. BOWMAN, M. C. BRADY, and C. V. PARKS, "Validation of the Scale System for PWR Spent Fuel Isotopic Composition Analyses," ORNL/TM-12667, Oak Ridge National Laboratory (March 1995).

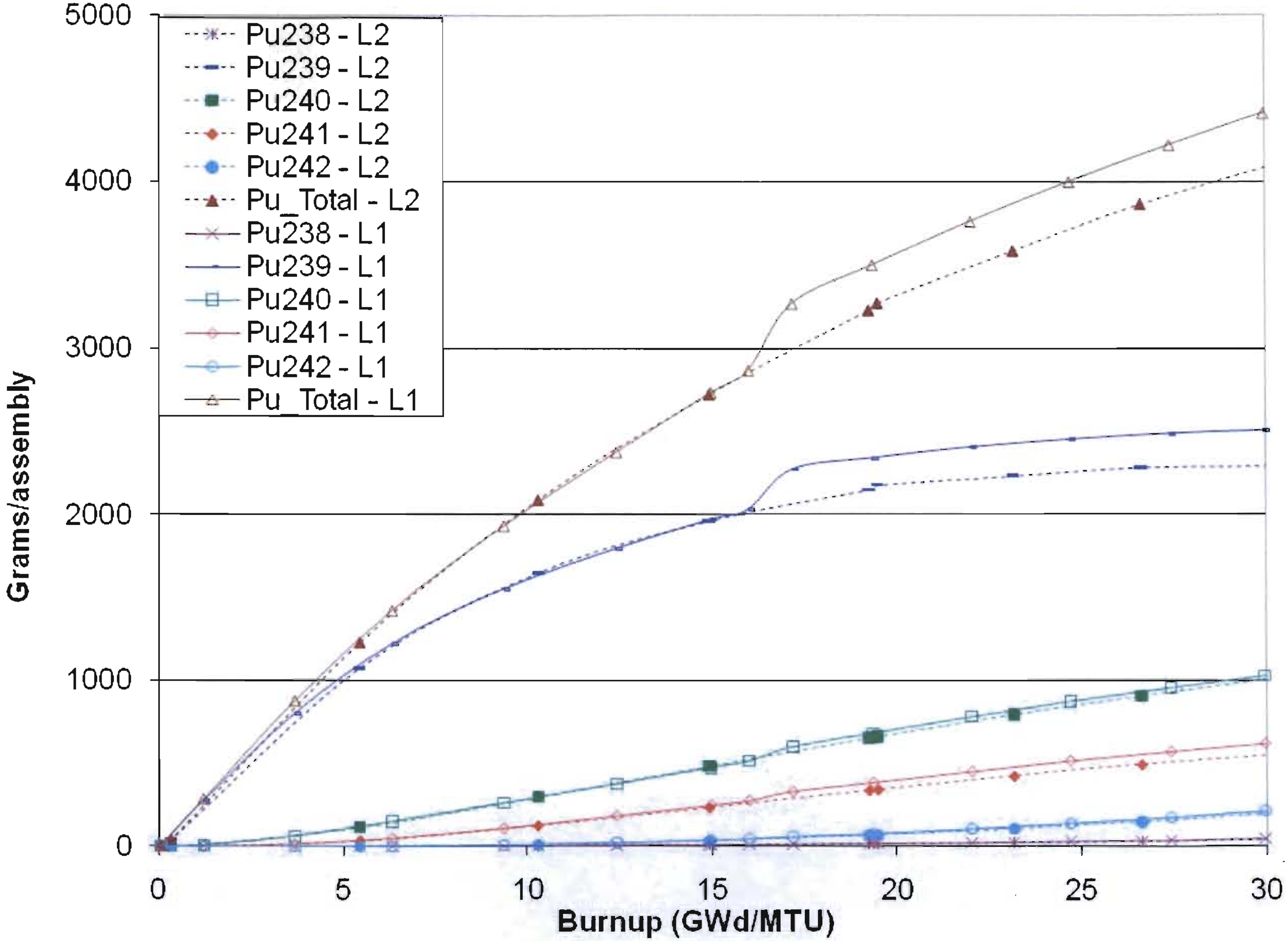
Relative Percent Error Code Comparison



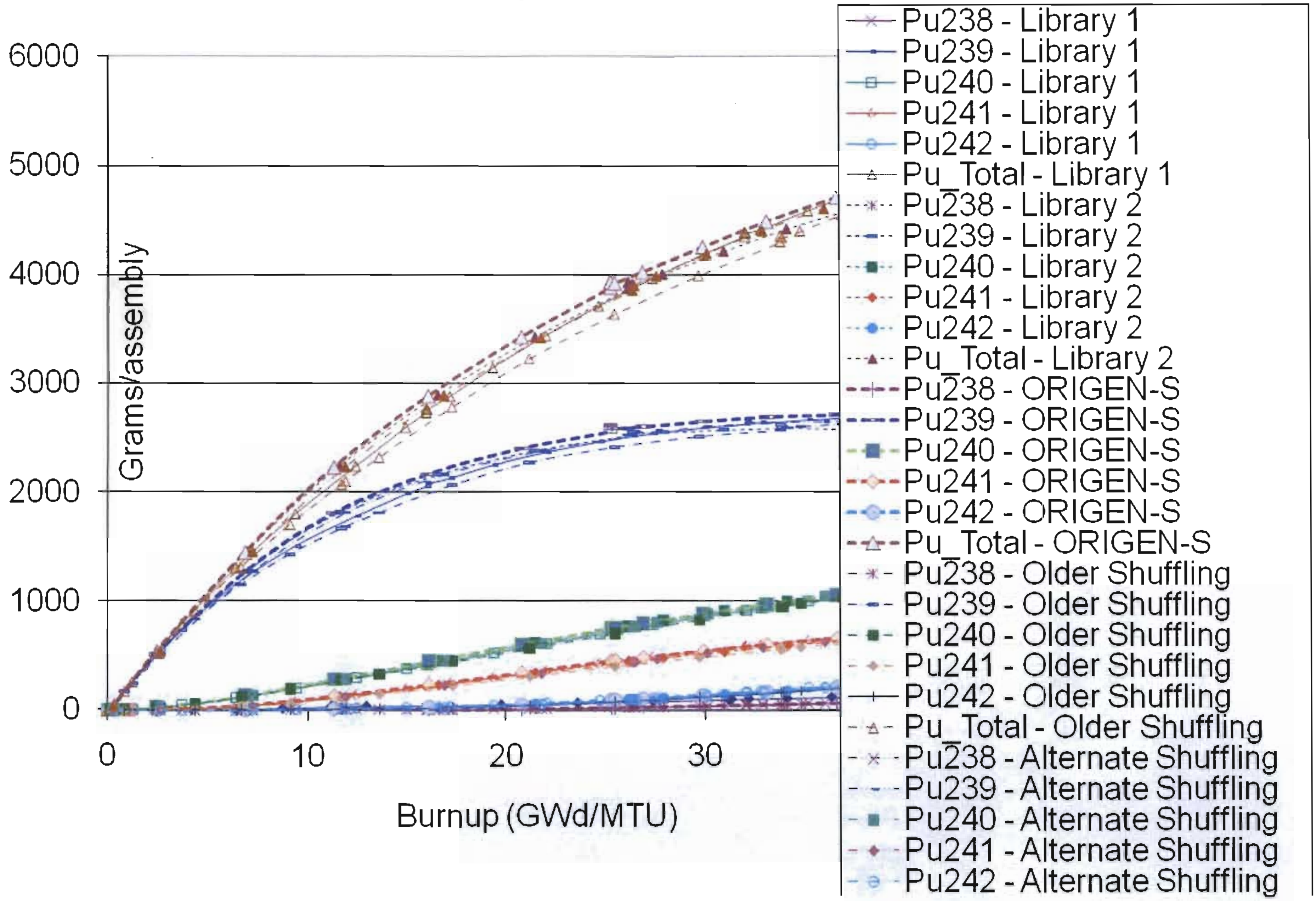
Plutonium Isotopic Correlations for 2wt%



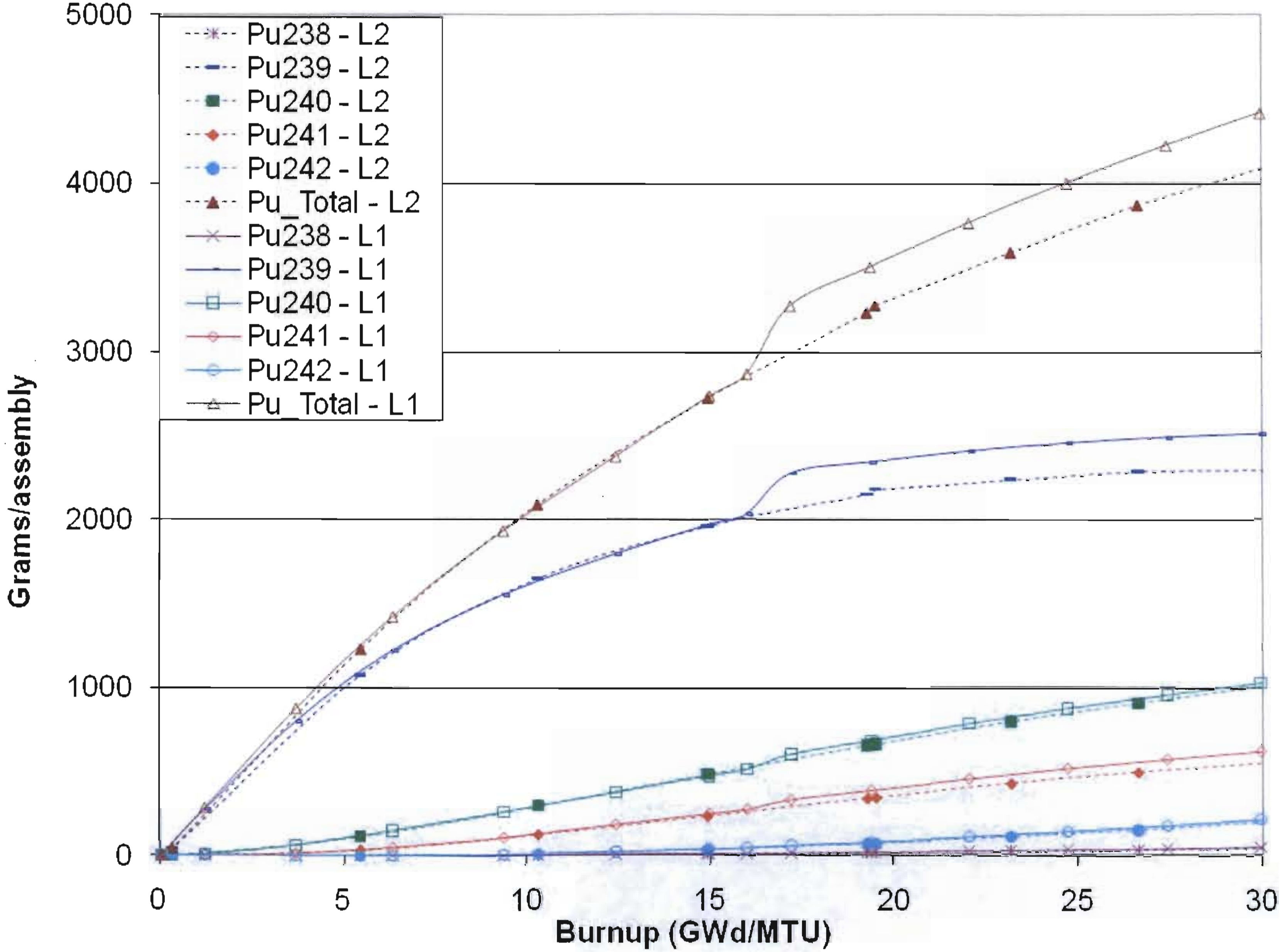
Plutonium Isotopic Correlations for 3wt%



Plutonium Isotopic Correlations for 4wt%

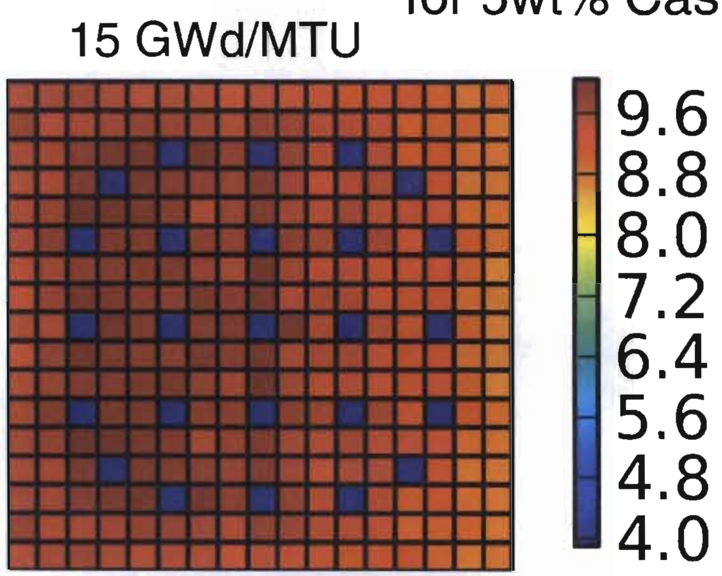


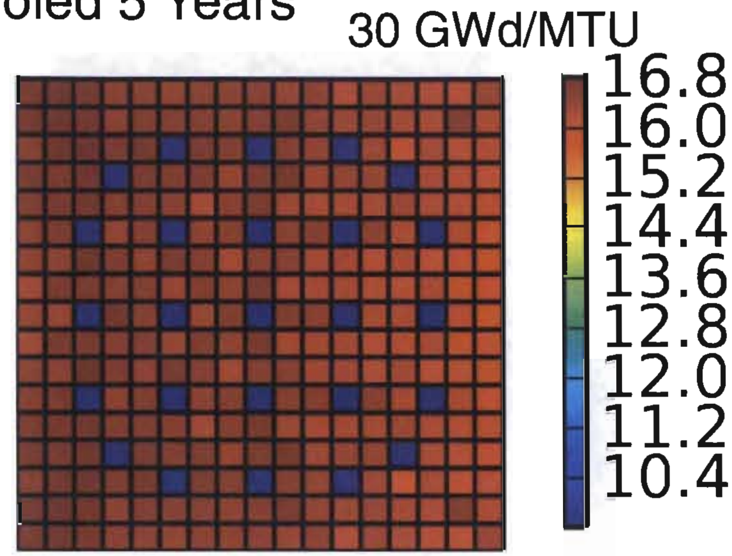
Plutonium Isotopic Correlations for 5wt%

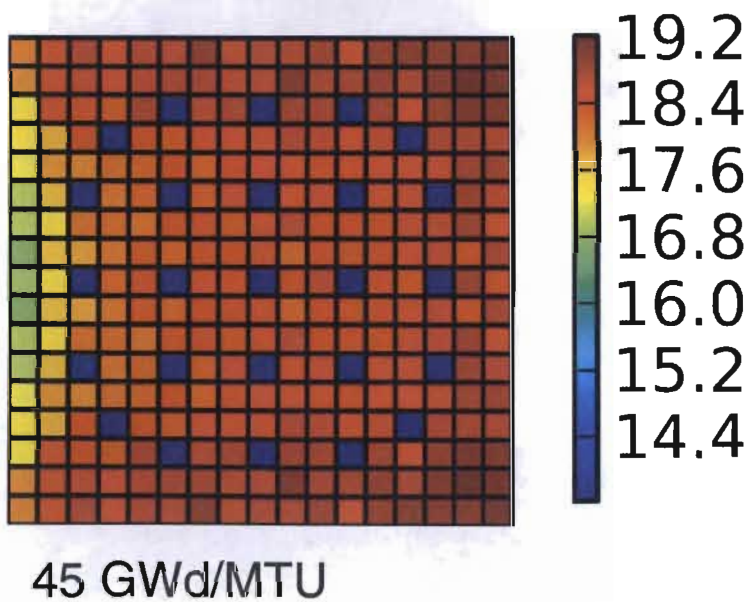


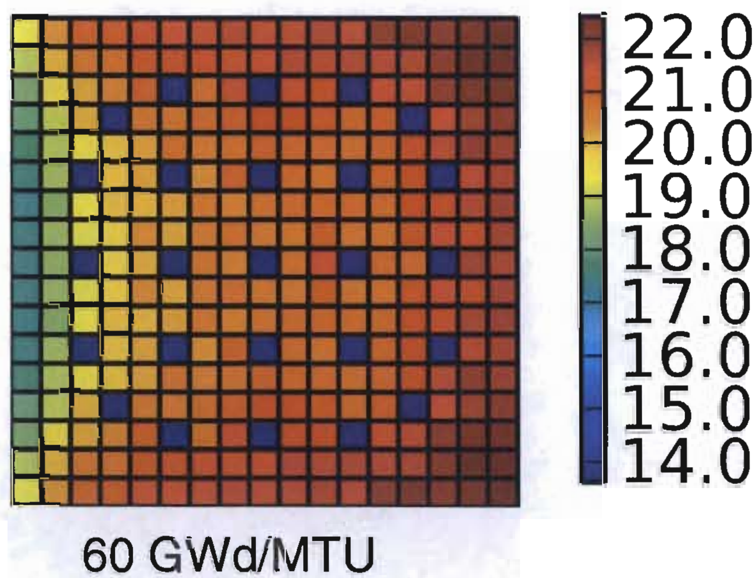
Change in Pu Content With Burnup

for 5wt% Cases Cooled 5 Years



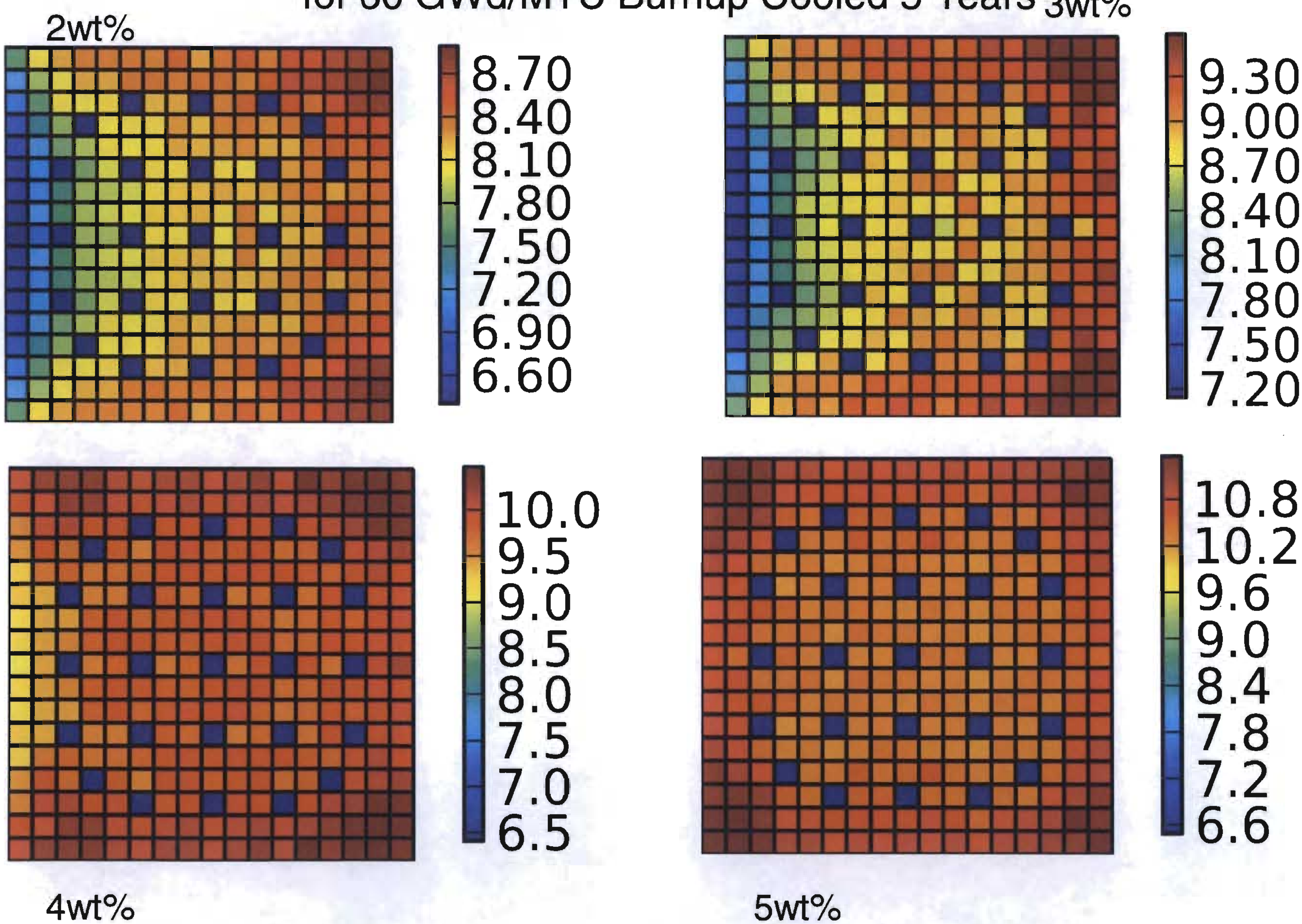






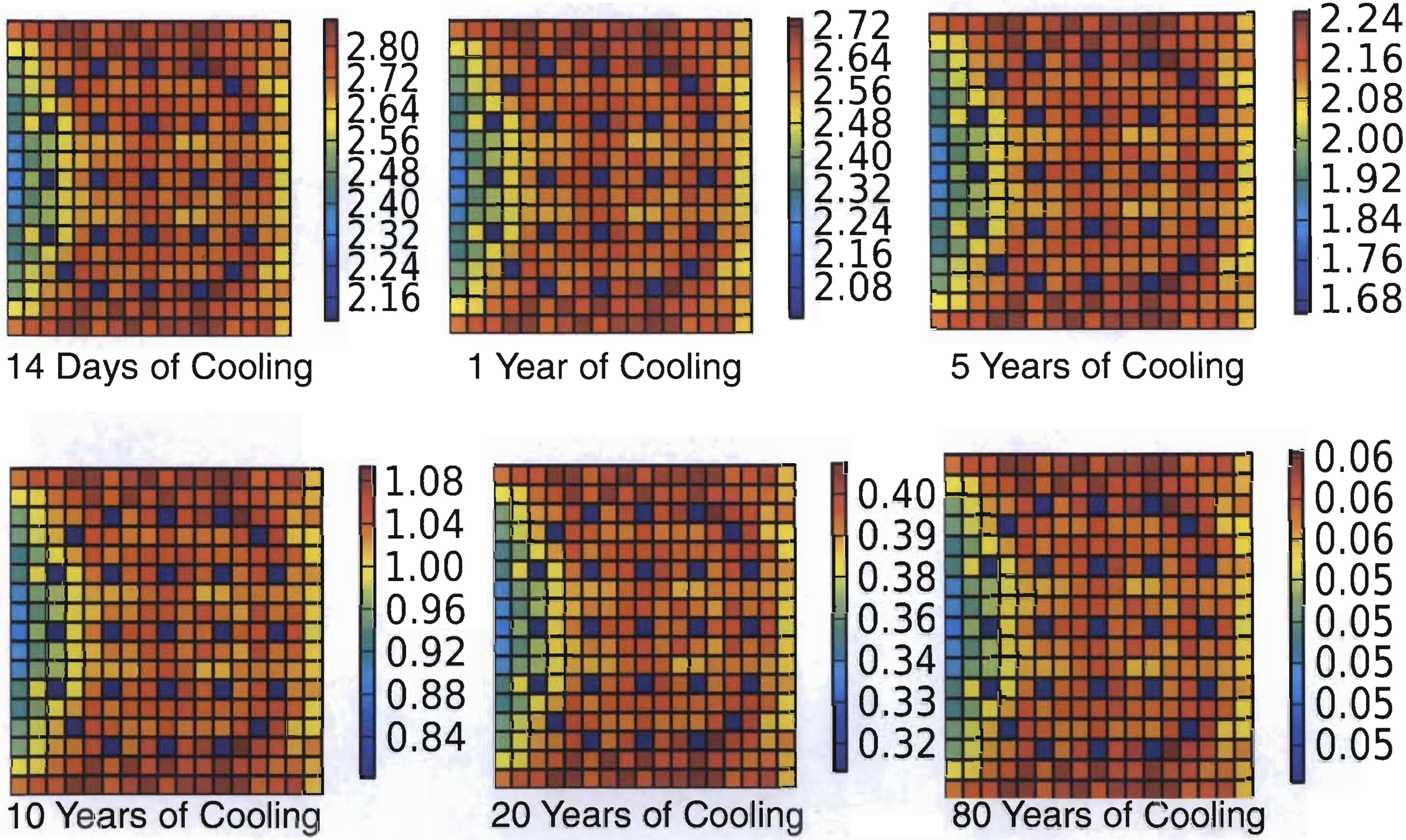
Change in ^{239}Pu with Enrichment

for 30 GWd/MTU Burnup Cooled 5 Years



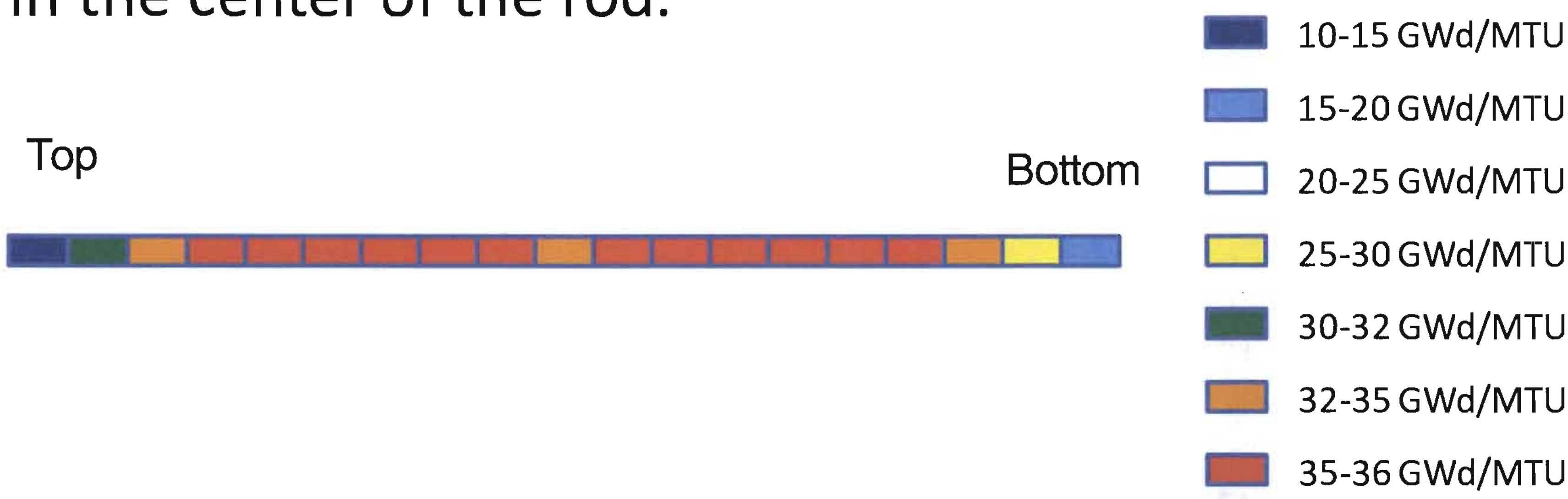
Change in ^{241}Pu with Cooling Time

for 45 GWd/MTU Burnup, 4wt% Enriched



Axial Burnup Profile

- The fuel was modeled as all one region axially.
- In reality, a burnup distribution such as that below would be observed.
- Measurements could consistently take place in the center of the rod.

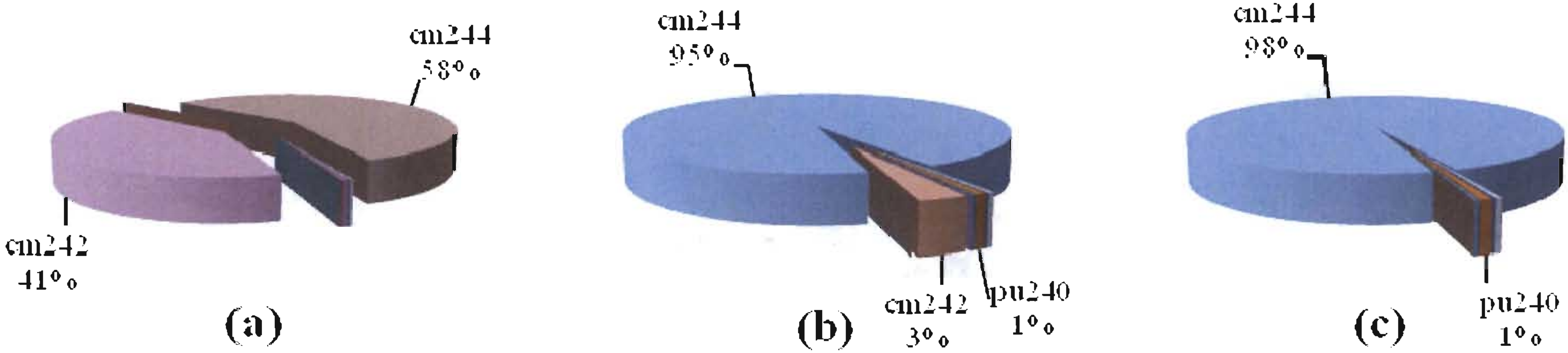


Conclusions

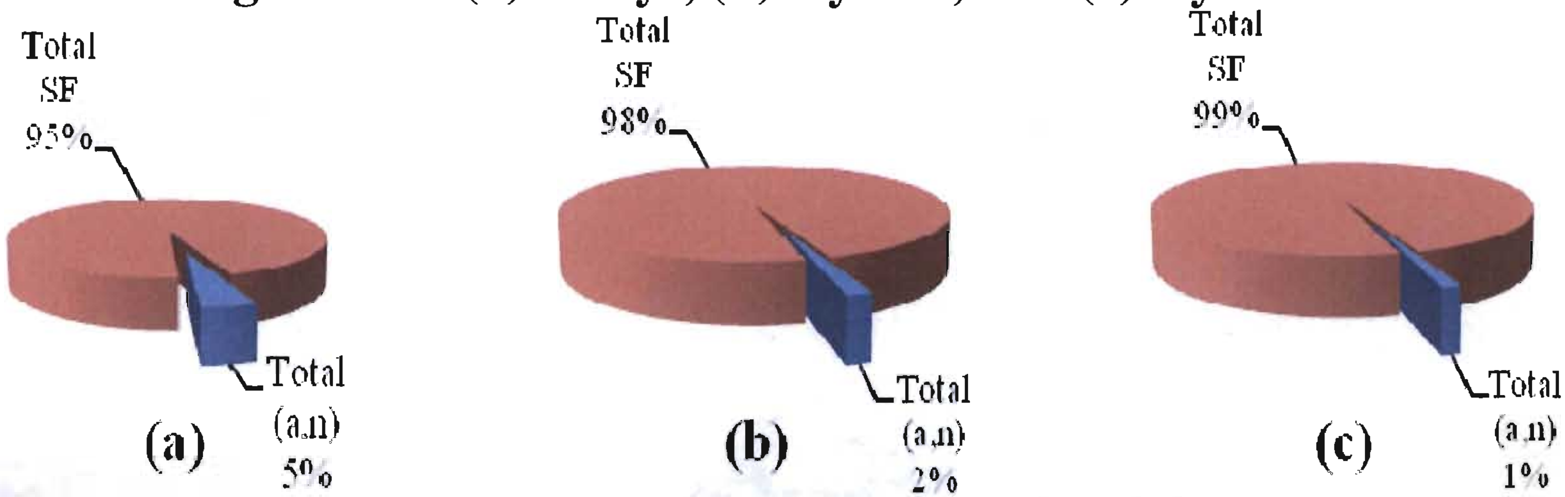
- The first library yields valuable information about the effect of burnup, initial enrichment, and cooling time on various detectors.
- The second library gives more realistic burnup fluctuations for PWR assemblies for detector analyses.
- The third library will provide a set of data for additional sensitivity studies.
- Monte Carlo burnup calculations have been benchmarked for low BU, low IE conditions and perform well!

Additional Slides

Neutron Source Term

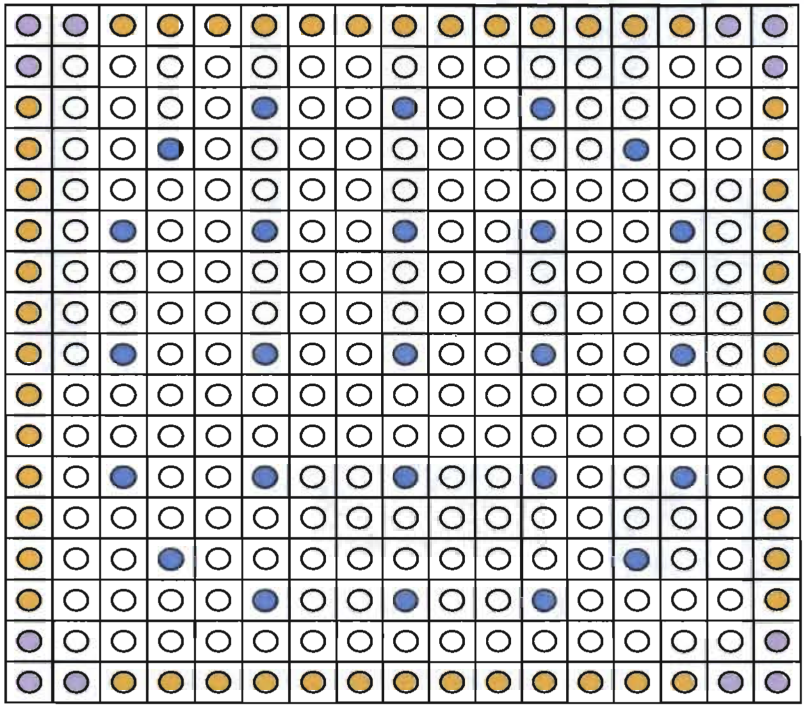


Spontaneous Neutron Contributors for 30 GWd/MTU, for cooling times of (a) 7 days, (b) 2 years, and (c) 5 years.



Neutron signal component contributors for 5-year CT at:
(a) 15 GWd/MTU, 2 w%, (b) 30 GWd/MTU, 3 w%, and (c) 45 GWd/MTU, 4 w%

Position of Control/Shutdown Rods and Burnable Poisons



○ = Fuel Rod

● = Wet Annular Burnable Absorber Or Guide Tube

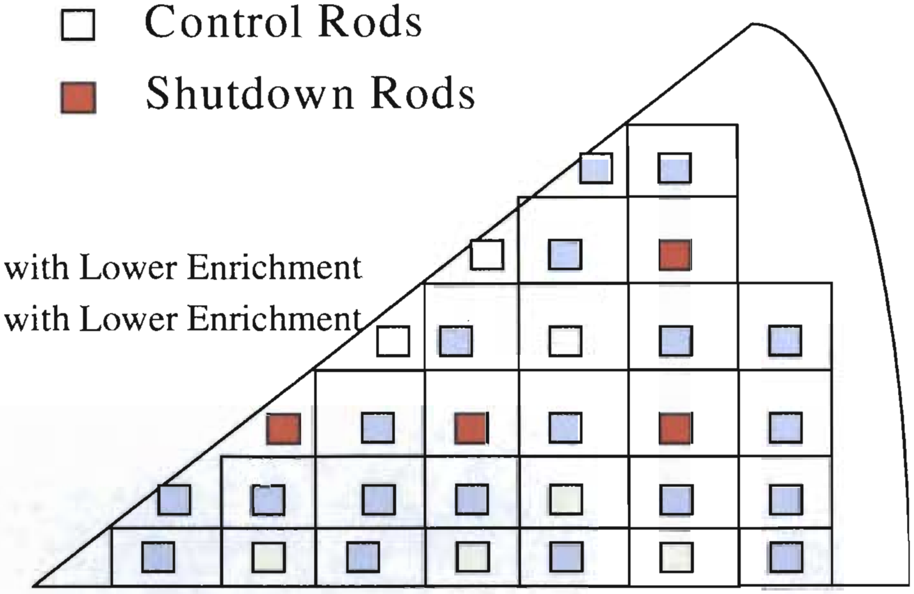
○ = Fuel Rod with Lower Enrichment

○ = Fuel Rod with Lower Enrichment

□ No Shutdown/Control Rods

□ Control Rods

■ Shutdown Rods



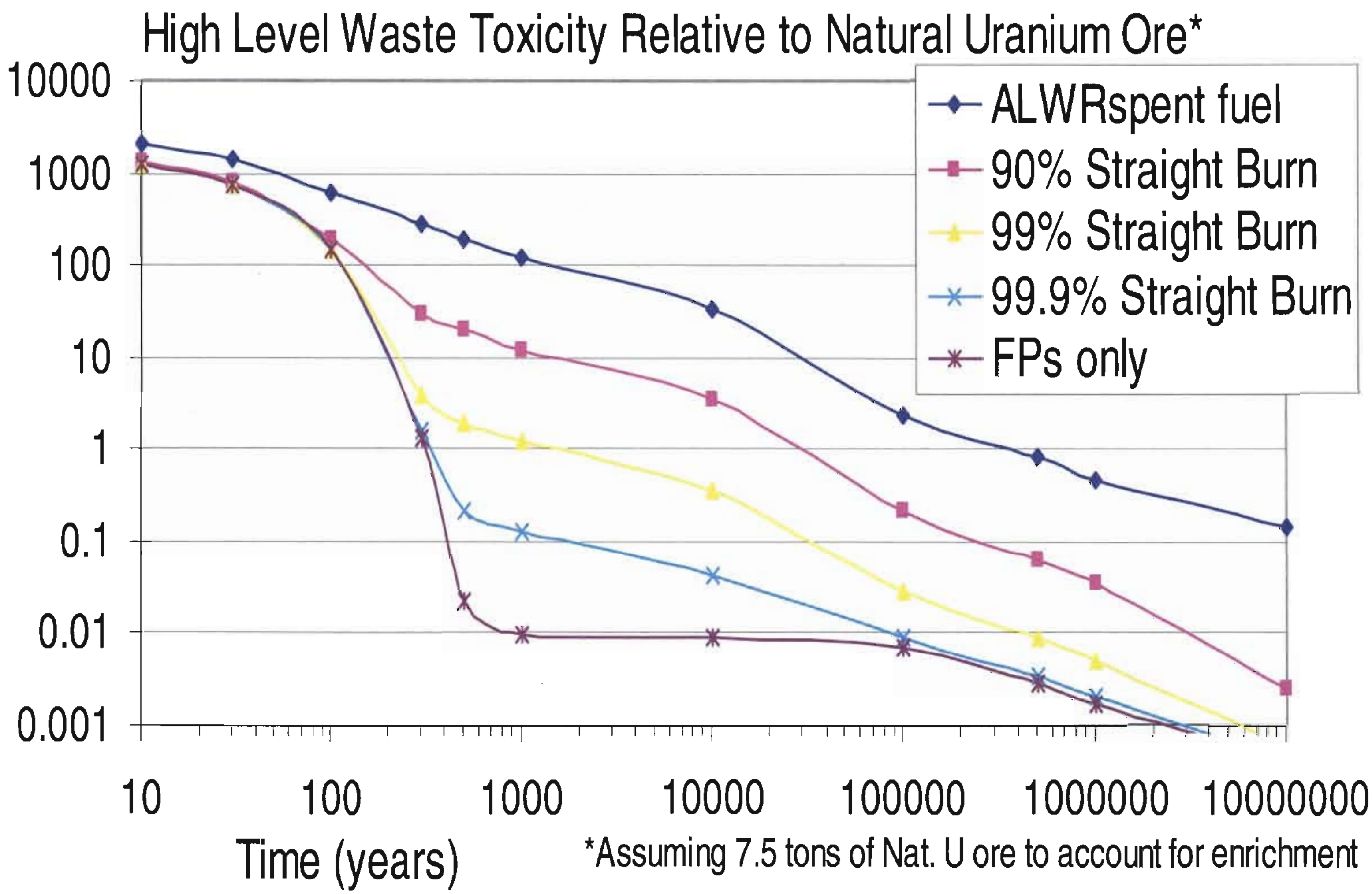
Time Steps for 2 and 3 wt% Cases

Step #	Time Step (d)	Position 1	Position 2	Cumulative
1	0.5	0.0034	–	19.3
2	4	0.3	0.2	19.5
3	75	5.3	3.8	23.1
4	75	10.1	7.4	26.7
5	75	14.7	10.9	30.2
6	75	19.3	14.2	33.5

Time Steps for 5 wt% Case

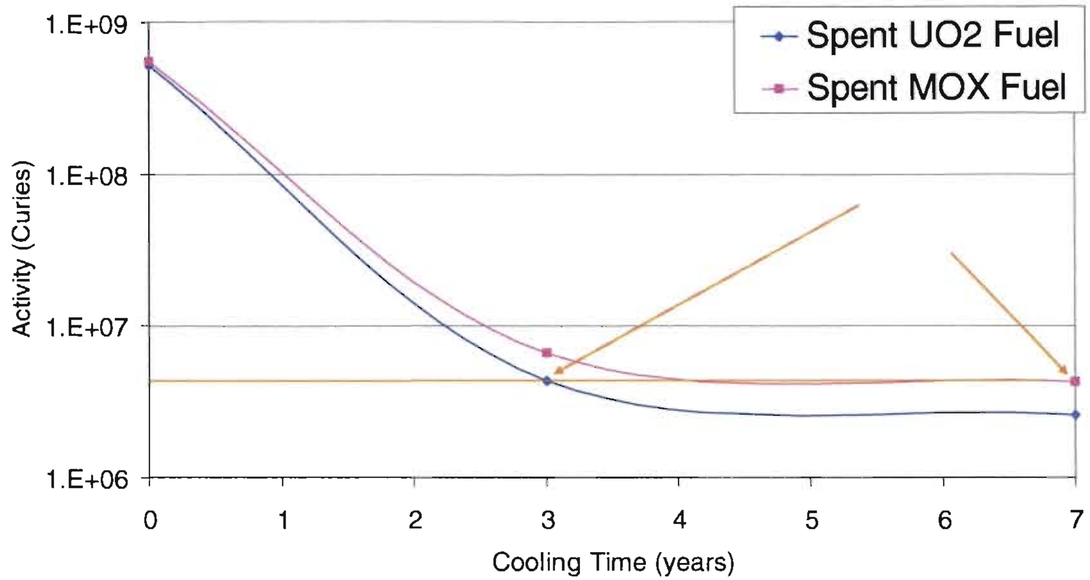
Step #	Time Step (d)	Position 1	Position 2	Cumulative	Position 3	Cumulative
1	0.5	0.004	–	36.3	–	60.2
2	4	0.3	0.2	36.5	–	60.2
3	80	5.96	3.9	40.2	0.2	60.4
4	80	11.4	7.4	43.7	0.4	60.6
5	80	16.6	10.8	47.1	0.7	60.9
6	80	21.7	14.1	50.4	1.0	61.2
7	80	26.7	17.4	53.7	1.4	61.6
8	80	31.6	20.7	57.0	1.9	62.1
9	80	36.3	23.9	60.2	2.4	62.6

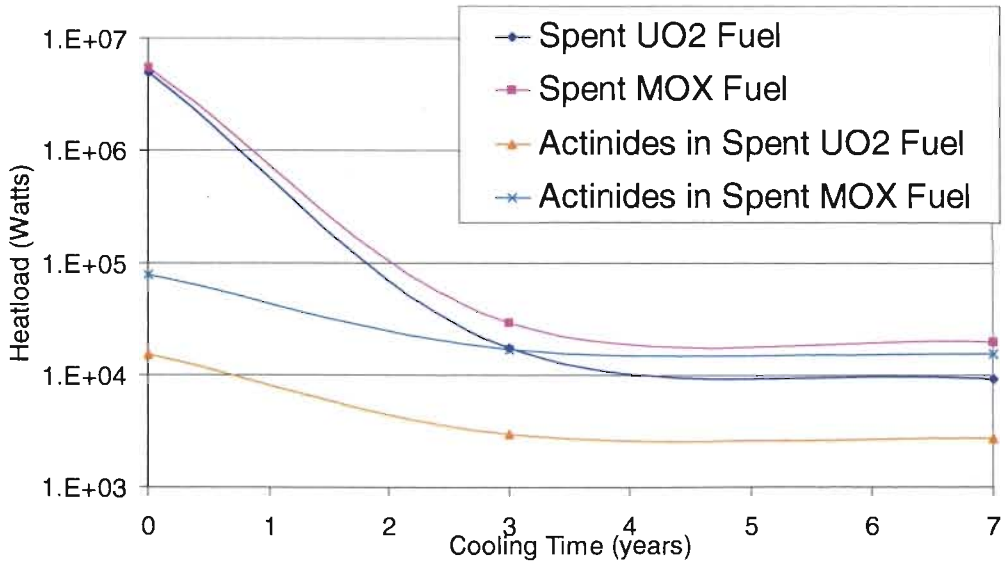
Radiotoxicity of Spent Fuel



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