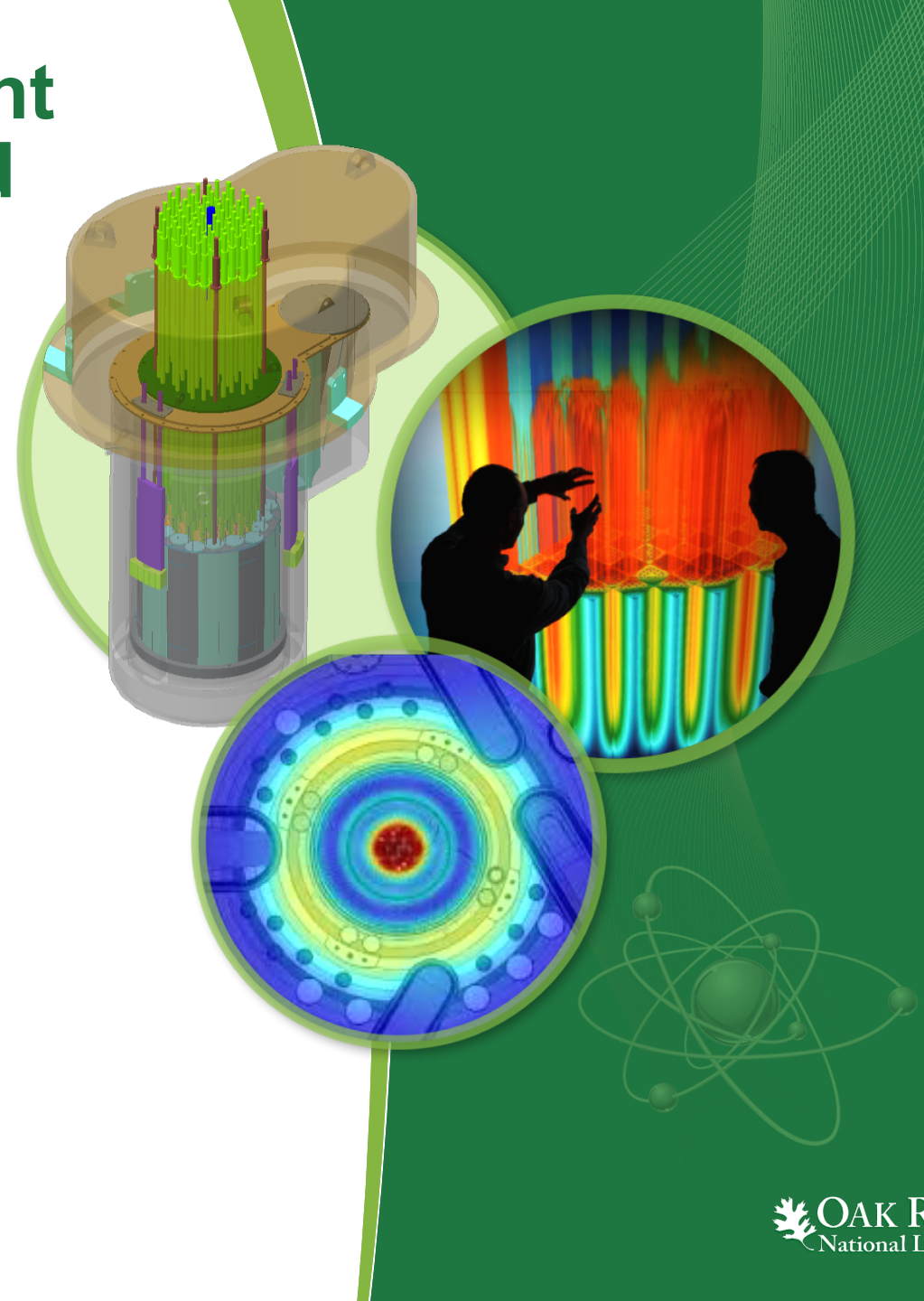


High-Fidelity Modeling of Spent Fuel Assemblies for Advanced NDA Instrument Testing

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¹Oak Ridge National Laboratory; ²Lawrence Livermore National Laboratory; ³Los Alamos National Laboratory; ⁴European Commission, DG Energy, EURATOM; ⁵Swedish Nuclear Fuel and Waste Management Company (SKB);

SCALE Users' Group Workshop, Sep. 2017



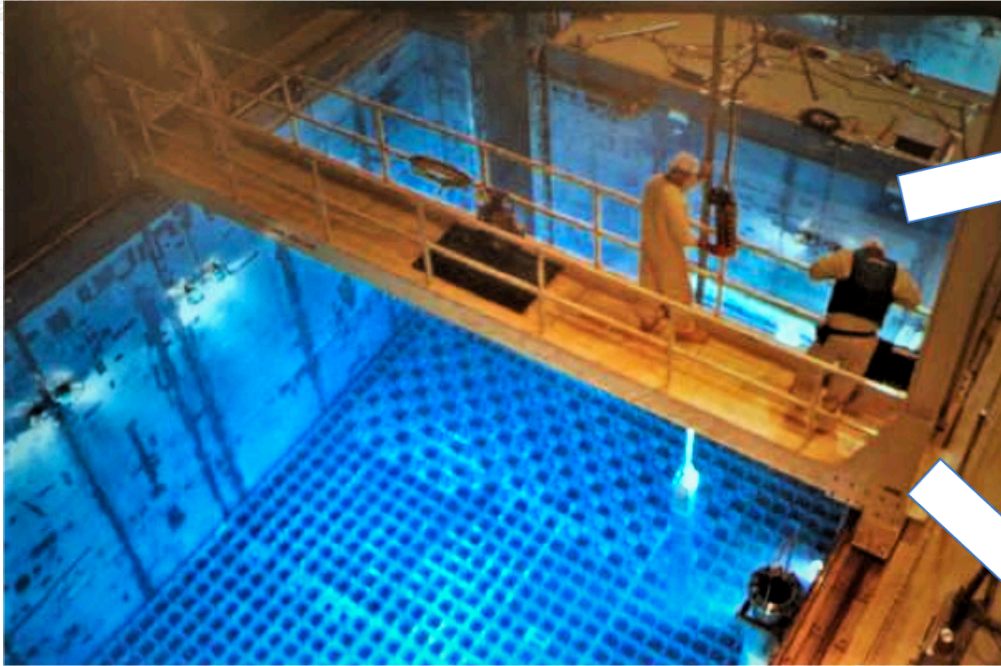
Outline

- Background of the Spent Fuel NDA project
- High-fidelity burnup modeling needed for spent fuel analysis
 - Complex nuclide composition and radiation source terms in spent fuel
- A new interface for 3D fuel assembly burnup calculations
 - ORIGAMI
- Verification of calculation results
 - Gamma spectra, decay heat, and total Pu
- Summary

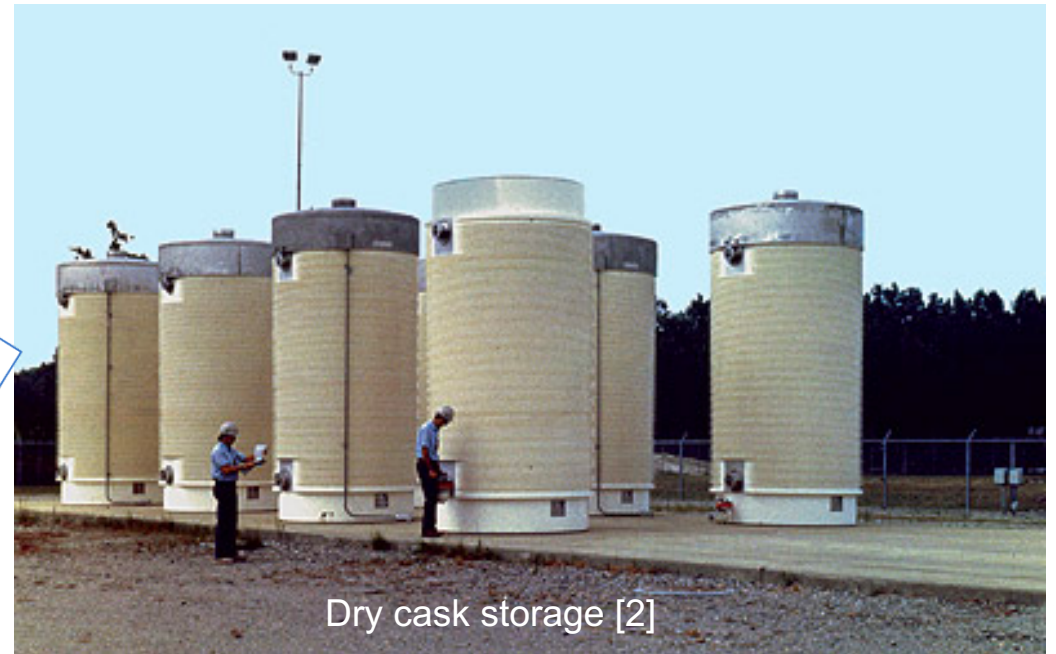
The Spent Fuel NDA (formerly NGSF-SF) project

- Driver: spent fuel assemblies contain ~1% Pu in their compositions.
- General purpose: strengthening the technical toolkit of safeguard inspectors by developing advanced nondestructive assay (NDA) technologies for spent nuclear fuel measurements.
- The technical goals: detect partial defects (missing/replaced fuel pins); verify operator declarations; estimate Pu mass; estimate reactivity; estimate decay heat.
- Three main phases, and we are now at Phase III:
 - Measurements for Characterization and Validation. Integrate two or more complementary techniques into a few systems. Fabrication of prototype NDA instruments. Field-testing of spent fuel in Sweden, South Korea, and Japan;
- Multi-year, and multi-institution project involving LANL, ORNL, LLNL, SKB, EURATOM, KAERI, and several others.
- NDAs tested (or to be tested): Passive Neutron Albedo Reactivity (PNAR), Self-integration Neutron Resonance Densitometry (SINRD), ^{252}Cf Interrogation with Prompt Neutron (CIPN), Passive Gamma, Differential Die-Away Self-Interrogation (DDSI), Differential Die-Away (DDA)

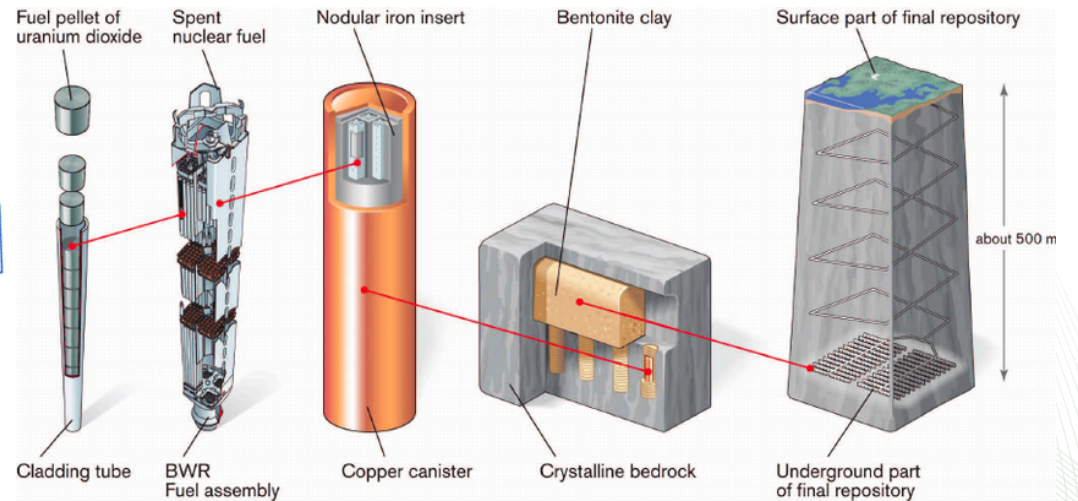
Partial defect tests are required before spent fuel assemblies being transferred to “difficult-to-access” storage.



Spent fuel storage pool [1]



Dry cask storage [2]

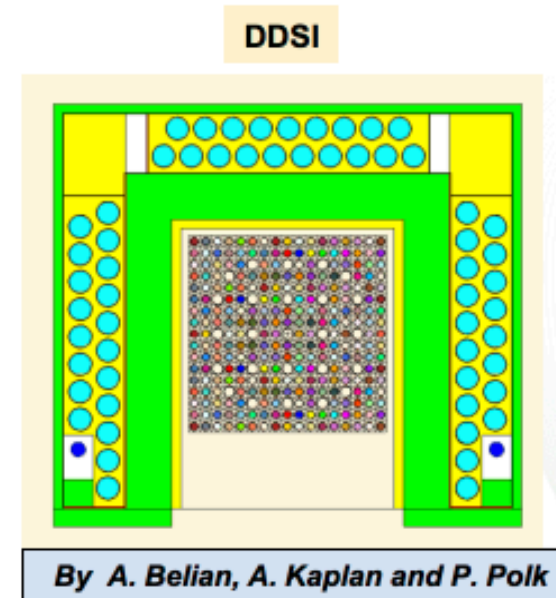
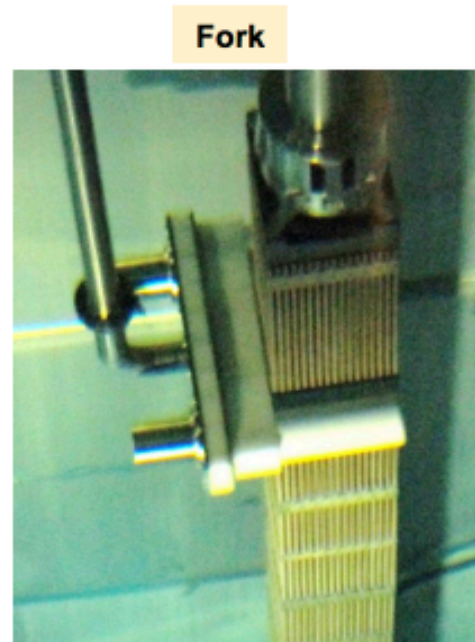
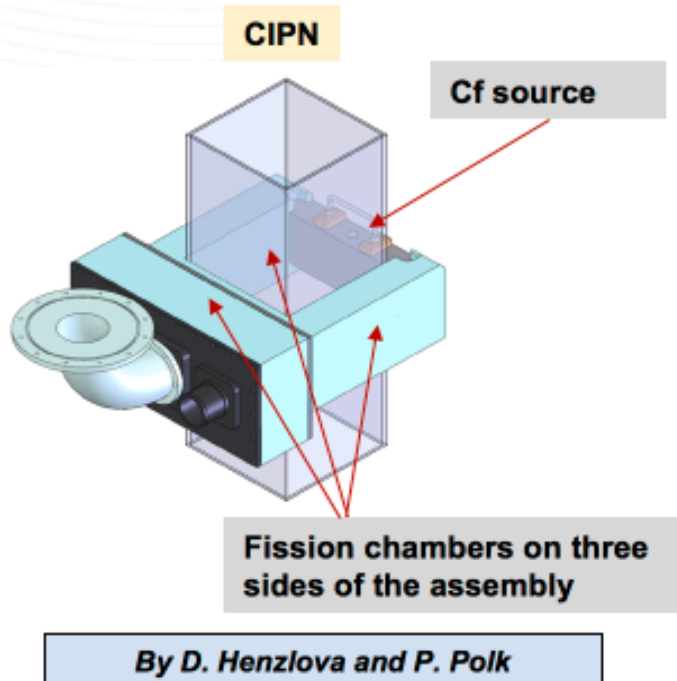


Encapsulation and final disposal [3]

[1]: <https://www.linkedin.com/pulse/performance-improvement-case-study-1-outage-duration-todd-mccann>
[2]: <https://www.nrc.gov/reading-rm/doc-collections/fact-sheets/dry-cask-storage.html>
[3]: https://www.researchgate.net/publication/260877239_The_Use_of_Clay_as_an_Engineered_Barrier_in_Radioactive-Waste_Management_-_A_Review/figures?lo=1

NDA testing/measurement with spent fuel

- Testing of (PNAR) and SINRD on Fugen Fuel (irradiated MOX) in 2013 in Japan.
- Testing of CIPN and SINRD on several PWR spent fuel assemblies in 2013 in Republic of Korea (ROK).
- Passive gamma measurement on **25 PWR** and **25 BWR** spent fuel assemblies (SKB-50) in 2013 and 2014 in **Sweden**.
- Fork measurement with SKB-50 in 2014 and 2015.
- Testing of DDSI and DDA with SKB-50 is planned for the next couple years.

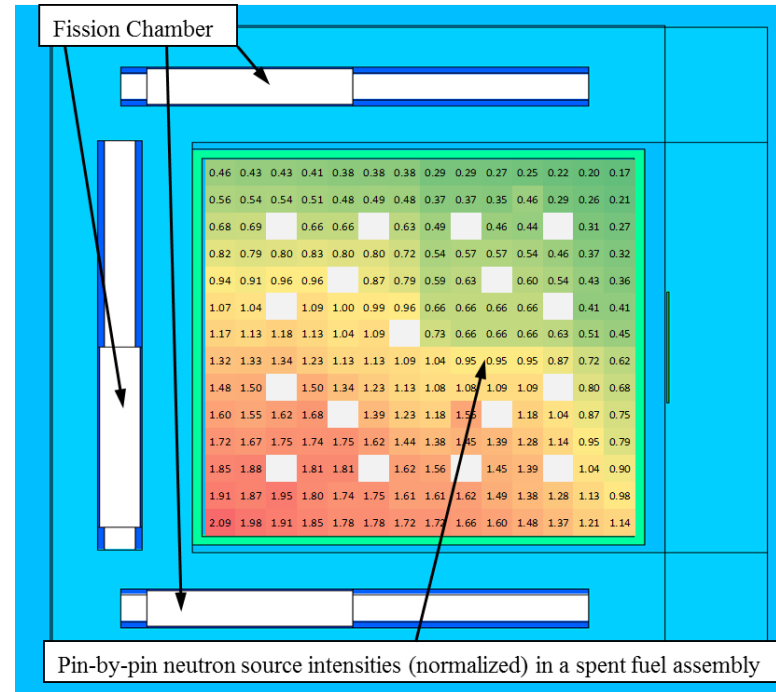


Why is high-fidelity spent fuel modeling and simulation needed?

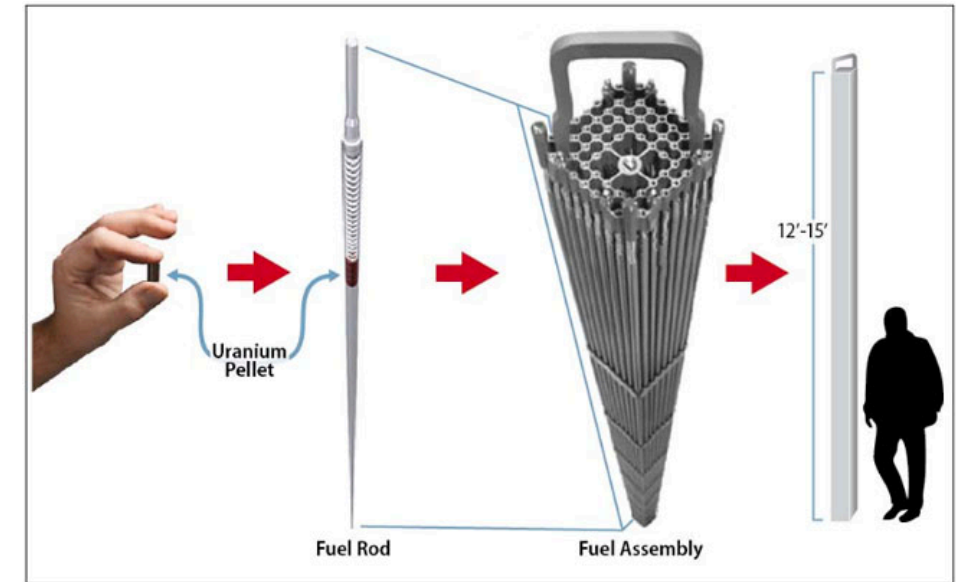
- Detailed nuclide compositions and spatial distribution are needed for 3D NDA modeling and simulation, in order to quantify instrument performance.
- Calculations provide a) the correlations between observed measures and the quantities of interest not directly measured and b) verification for measurements since the actual assembly inventories cannot be measured.

28.2	27.8	27.5	27.3	27.1	27.0	26.9	25.4	25.3	25.0	24.6	24.0	23.2	22.3
29.6	29.5	29.7	29.1	28.8	29.2	28.7	27.1	27.4	26.8	28.3	26.0	24.8	23.6
31.0	31.4	31.3	31.1	30.7	29.0	28.8	28.3	26.5	24.8				
32.1	32.2	32.8	32.5	32.8	32.5	31.5	29.6	30.3	30.2	29.3	28.7	27.2	25.8
33.2	33.4	34.0	34.2	33.4	32.4	30.1	30.9	30.7	29.7	28.1	26.7		
34.3	34.9	35.0	34.5	34.0	34.0	30.9	30.9	31.3	31.2	28.2	27.4		
35.1	35.2	35.7	34.9	34.4	34.9	31.8	31.0	30.9	30.9	30.7	29.3	27.9	
36.2	36.3	36.8	35.9	35.2	34.9	35.0	34.4	33.8	33.6	33.5	33.3	31.7	30.3
37.0	37.7	37.8	37.8	37.0	35.8	35.0	34.7	34.8	35.2	35.1	32.8	30.9	
37.7	38.0	38.7	38.8	37.3	35.9	35.5	38.3	36.0	34.8	32.9	31.4		
38.5	38.7	39.4	39.0	39.2	38.6	37.2	36.8	37.6	37.3	36.2	35.4	33.6	32.1
39.2	39.9	39.8	39.5	38.6	38.2	37.7	37.0	34.8	32.9				
39.7	39.8	40.2	39.4	39.1	39.3	38.4	38.2	38.5	37.5	36.9	36.6	35.0	33.6
40.3	40.0	39.7	39.4	39.1	38.8	38.5	38.6	38.3	37.8	37.2	36.5	35.5	34.6

Pin-by-pin burnup map of a 14x14 spent fuel assembly



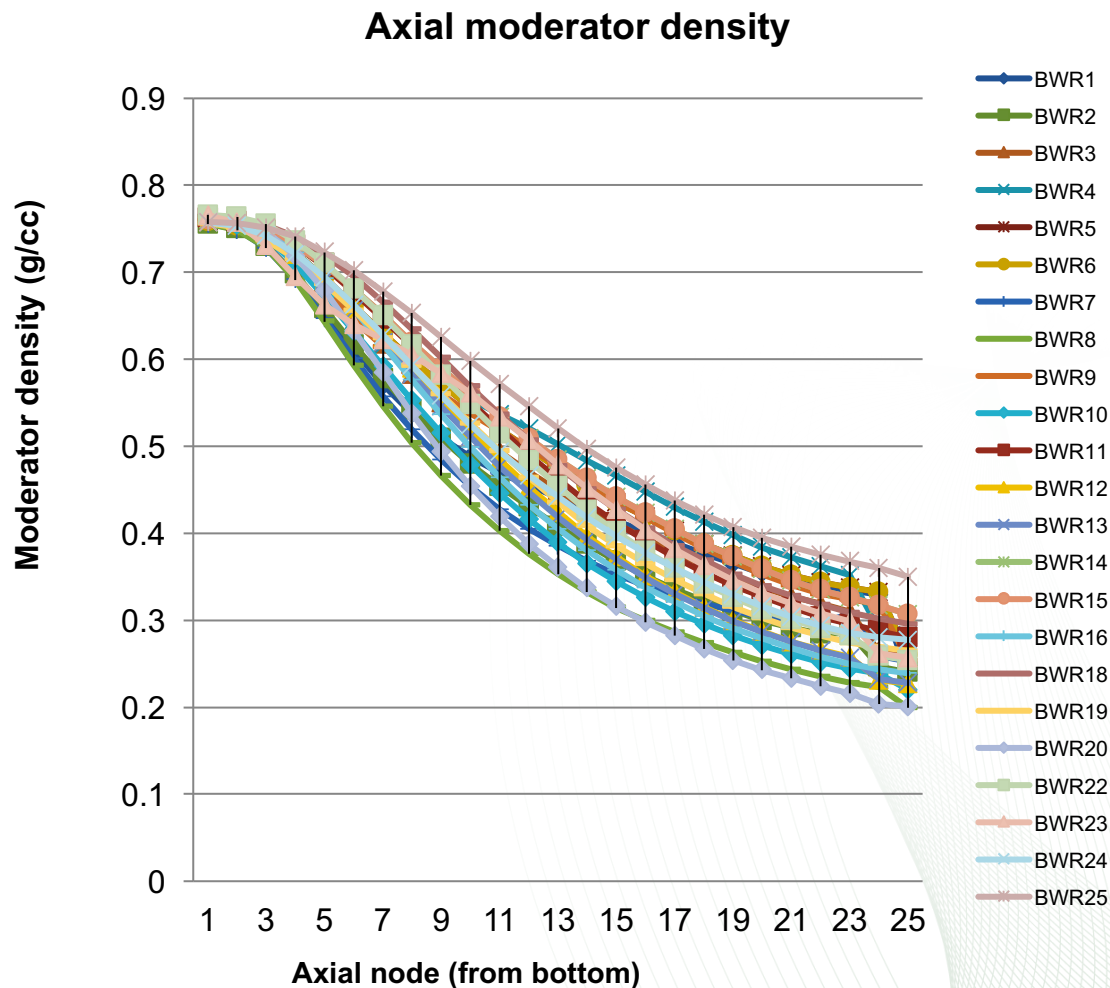
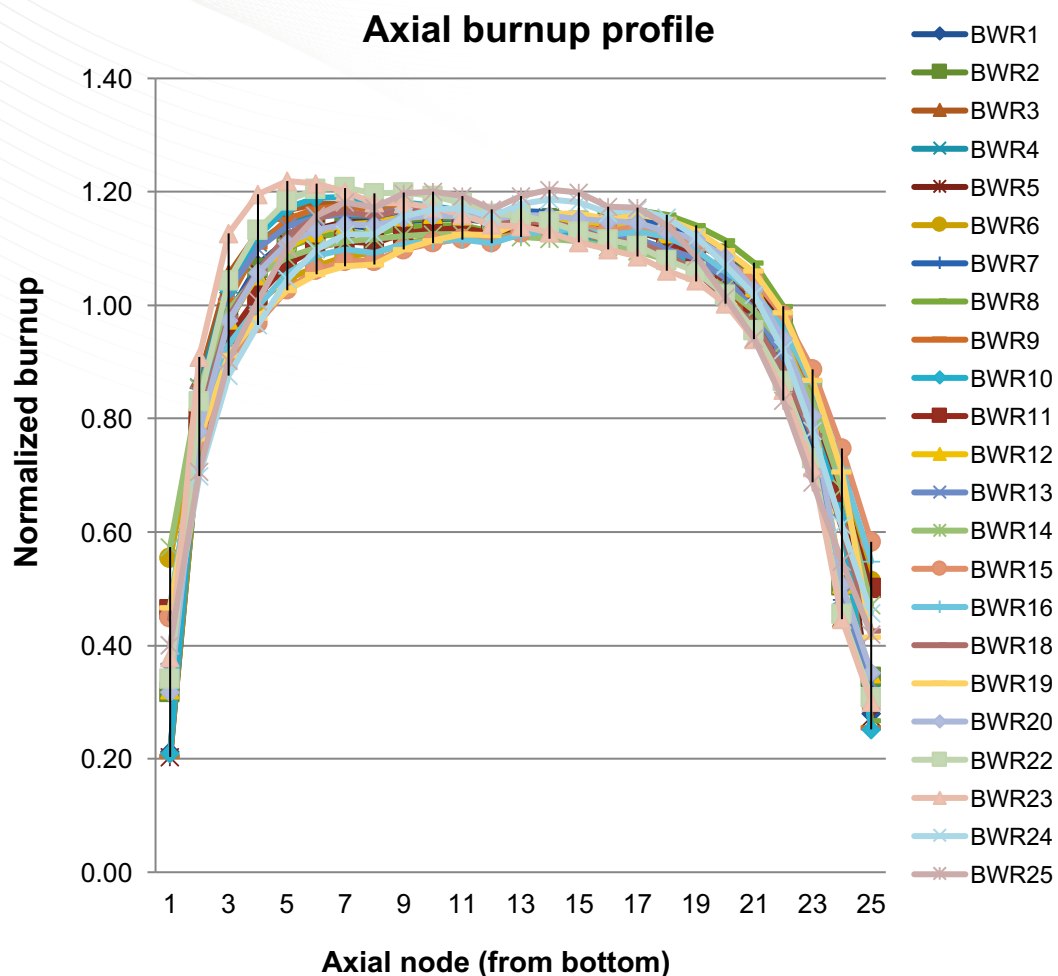
Neutron source distribution in the MCNP model for the CIPN detector



A fuel assembly [1]

Spent fuel is complicated...

Spent fuel contains hundreds of nuclides with varying compositions due to fuel designs, irradiation history, and irradiation conditions



Impact of Operator Uncertainty on Nuclide Concentrations

		Relative difference (%) in nuclide concentrations due to parameter <u>changes^a</u>					
Parameter	Uncertainty	²³⁹ Pu	total Pu	²³⁵ U	<u>total Fissile^b</u>	¹³⁴ Cs/ ¹³⁷ Cs	²⁴⁴ Cm
BPR exposure	empty vs. inserted	7.8	6.4	5.1	6.2	2.1	7.9
Boron concentration	±5%	0.6	0.4	0.3	0.4	0.2	0.7
<u>Gd rod exposure</u>	none vs. ⁴ <u>Gd^c</u>	1.9	1.9	1.8	1.9	0.0	1.8
Assembly burnup	±2.5%	0.3	2.1	7.4	4.1	4.5	22.6
Fuel Temp	±50K	1.2	0.9	0.7	0.9	0.2	0.4

^aThe maximum in each category is highlighted in red and bold.

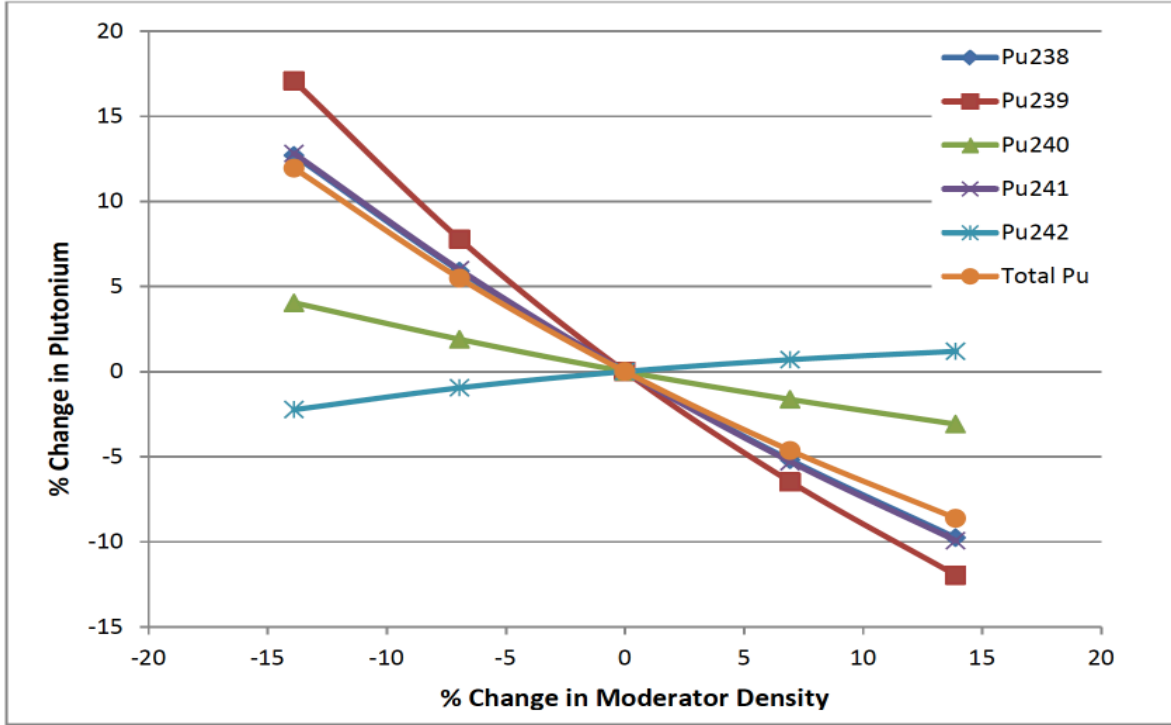
^bThese studies were based on the TMI-1 assembly NJ070G with a burnup of 45 GWd/tU, an initial enrichment of 4.6% and a cooling time of 5 years.

^cCombined mass of ²³⁵U, ²³⁹Pu, and ²⁴¹Pu.

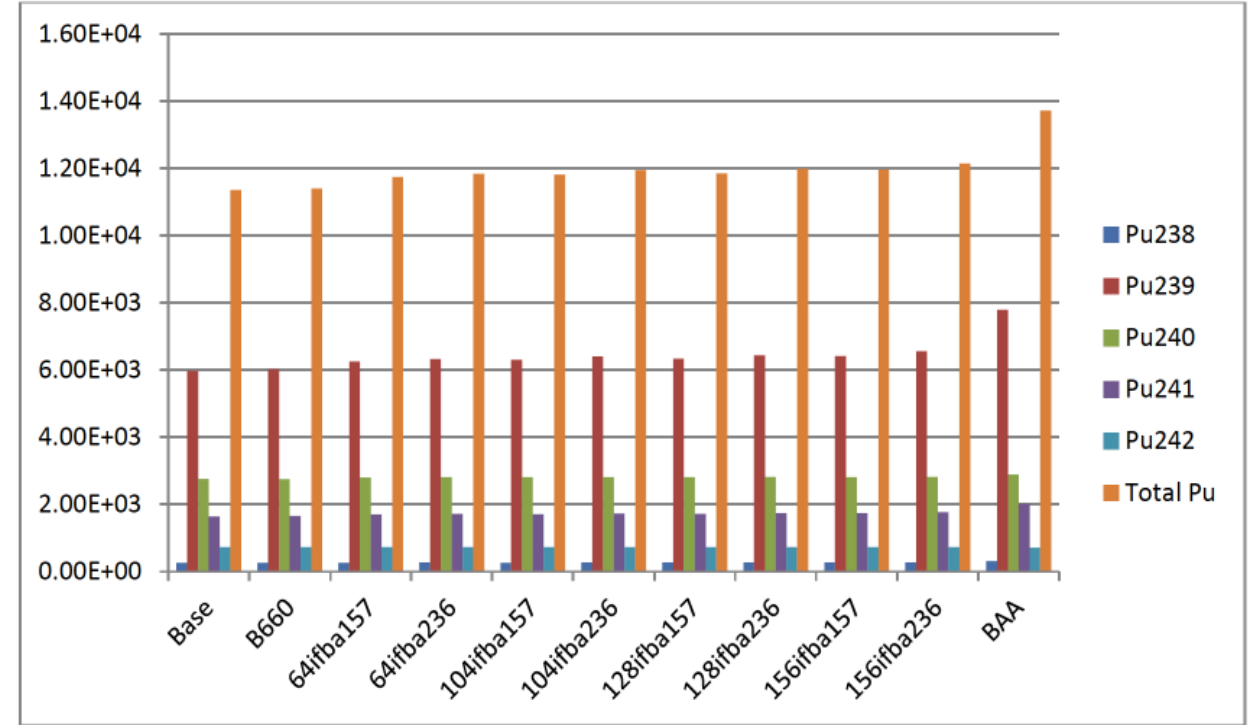
^dFor the TMI-1 assemblies, there are only 4 gadolinia (Gd) rods in total in one assembly.

- J. Hu, I. Gauld, J. Banfield, and S. Skutnik, "Developing Spent Fuel Assembly Standards for Advanced NDA Instrument Calibration – NGSF Spent Fuel Project," Oak Ridge National Laboratory report ORNL/TM-2013/576 (2014).

Sensitivity of Pu concentration



Sensitivity of Pu concentration to moderator density [1]

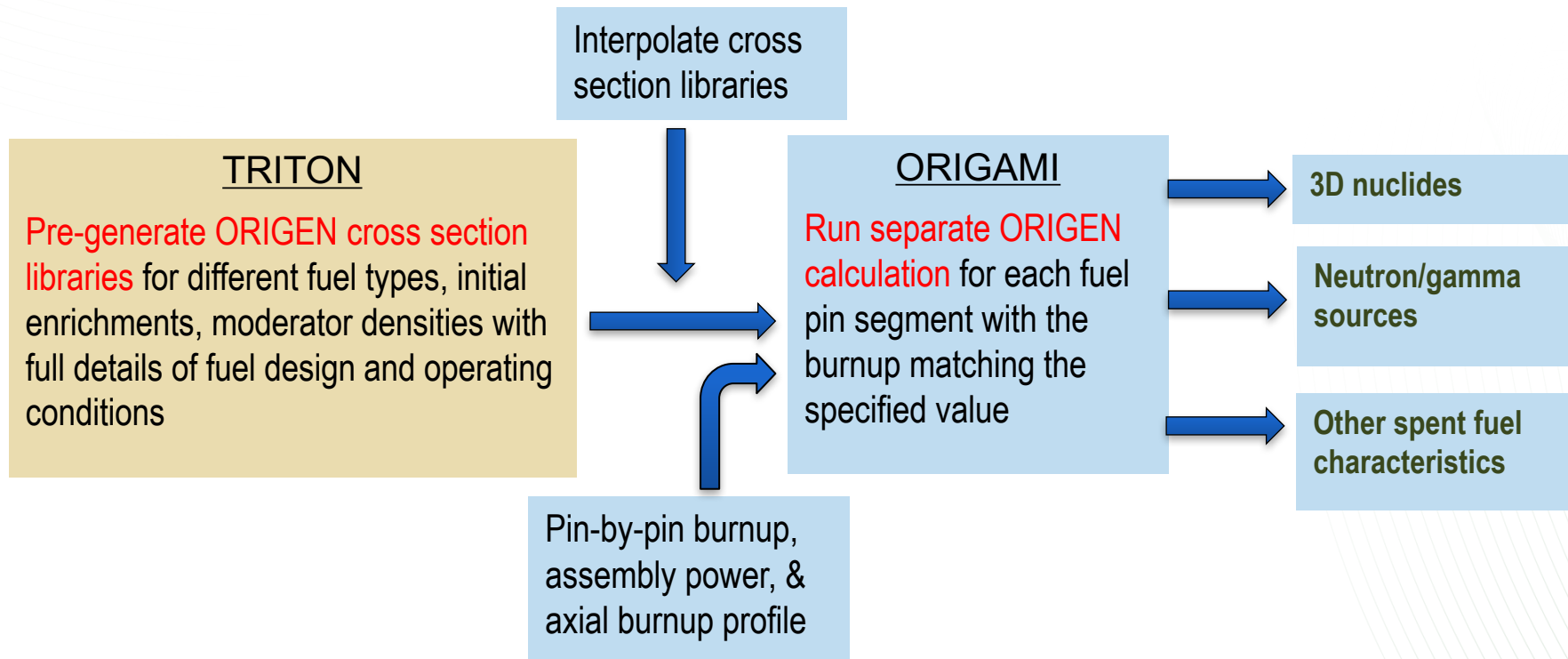


Sensitivity of Pu concentration to boron loadings in the fuel[1]

[1] B. Broadhead, I. Gauld, and et al., "Utilizing NGSF Spent Fuel Sensitivity Libraries to Estimate Model Uncertainties," in INMM Annual Meeting, Orlando, FL, 2012.

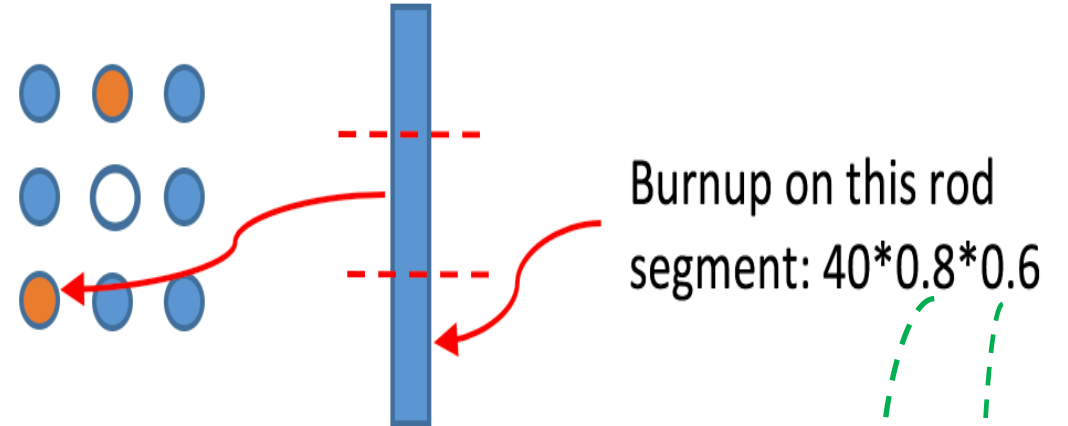
ORIGAMI: an automated ORIGEN interface for 3D fuel assembly burnup calculation

- A customized user interface of ORIGEN for 3-D assembly burnup calculations.
- Pre-generated cross-section libraries are interpolated to produce accuracies similar to full SCALE/TRITON simulations.
- Can generate nuclide compositions and decay heat for each axial node of each fuel pin based on specified burnup values.
- Accepts different compositions, enrichments, burnup, cross-section libraries for each fuel rod.



An example

```
1 =origami
2 title= 'multi-pin; multi-library'
3 options{ mtu=0.45 decayheat=yes mcnp=yes relnorm=no}
4 nonfuel= [ cr=3.5 fe=6.3 ]
5
6 fuelcomp{
7   uox(fuel_2pct){ enrich=2 dens=10.42 }
8   uox(fuel_4pct){ enrich=4 dens=10.45 }
9   mix(1){ comps[fuel_2pct=100] }
10  mix(2){ comps[fuel_4pct=97.0 Gd203=3.0 ] }
11  compmap= [ 1 2 1
12             1 0 1
13             2 1 1 ]
14
15  libs=[ w17x17 w17x17_Gd ]
16  libmap=[ 1 2 1
17           1 0 1
18           2 1 1 ]
19
20  pxy=[ 0.9 1.1 0.9
21        1.2 0 1.2
22        0.8 1.1 0.9 ]
23  pz=[ 0.6 1.0 0.5 ]
24  meshz=[ 0 120 240 360 ]
25  modz=[ 0.75 0.73 0.71 ]
26
27  hist[
28    cycle{ power=30 burn=500 nlib=4 down=45 }
29    cycle{ power=50 burn=300 nlib=4 down=45 }
30    cycle{ power=25 burn=400 nlib=4 down=1825 }
31  ]
32  ggrp=[ 10e6 2e6 1e6 0.01]
33  ngrp=[ 20e6 1e6 1e5 0.025 ]
34 end
```



Lib1

Lib2*

Radial power/burnup profile

Axial power/burnup profile

Assembly avg. burnup:
40 GWd/MTU

Lib2*, not included in the SCALE package; need to be generated by the user for the Gd rods

ORIGAMI Output Files

*_AxialDecayHeat

```
2.78253E+02
5.89804E+02
2.17135E+02
```

*_MCNP_matls.inp

```
C Axial zone: 03, Pin: 008
C Zone mass (grams): 2.144858E+04
m803 1001 -8.598225E-09
      1002 -6.035635E-10
      1003 -2.526046E-08
      2003 -8.794443E-09
      2004 -3.262135E-06
      3006 -2.660487E-17
      3007 -7.905803E-18
      4009 -5.885097E-13
      5010 -6.966128E-17
      5011 -4.479028E-15
```

*_MCNP_neutron.inp

```
C Neutron source for axial zone 03, pin 001
C Total intensity (n/sec): 5.2826E+05
SI103      H  2.5000E-08  1.0000E-01  1.0000E+00  2.0000E+01
SP103      D  1.1249E-02  2.5571E-01  7.3304E-01
```

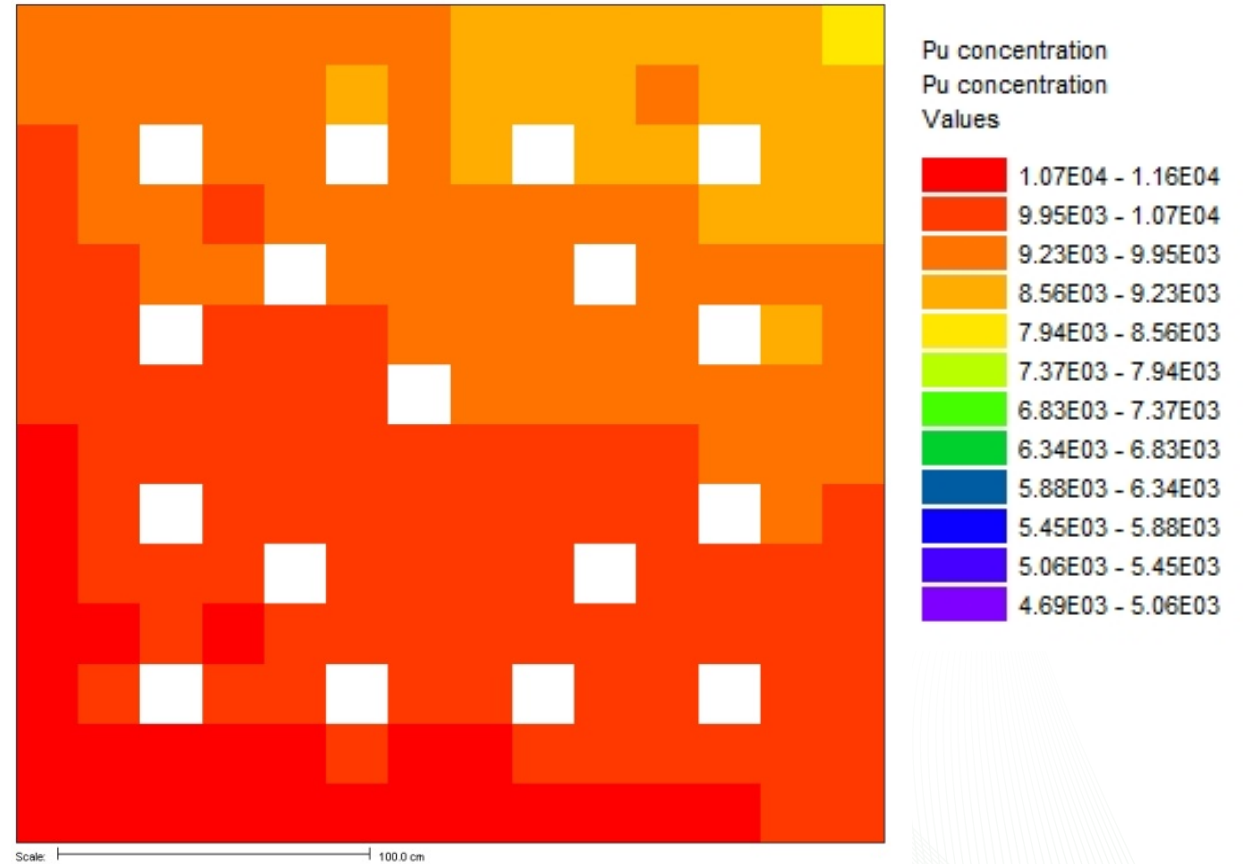
Much more info in the main output file "*.out"

```
=====
= Nuclide concentrations in grams, actinides for case 'axial zone: 001, pin: 03-01' (#6)
= multi-pin; multi-library
-----
(relative cutoff; integral of concentrations over time > 1.00E-04 % of integral of all
*)
      1290.000d  1290.093d  1290.278d  1290.834d  1292.503d  1297.510d  131
u-234      1.8117E+00  1.8117E+00  1.8117E+00  1.8118E+00  1.8119E+00  1.8122E+00  1.81
u-235      6.6208E+01  6.6208E+01  6.6208E+01  6.6208E+01  6.6208E+01  6.6209E+01  6.62
u-236      5.0132E+01  5.0132E+01  5.0132E+01  5.0132E+01  5.0133E+01  5.0133E+01  5.01
u-238      1.7853E+04  1.7853E+04  1.7853E+04  1.7853E+04  1.7853E+04  1.7853E+04  1.78
np-237      6.2240E+00  6.2248E+00  6.2263E+00  6.2307E+00  6.2425E+00  6.2679E+00  6.29
pu-238      2.7486E+00  2.7491E+00  2.7500E+00  2.7527E+00  2.7589E+00  2.7694E+00  2.78
pu-239      9.3958E+01  9.3987E+01  9.4044E+01  9.4197E+01  9.4530E+01  9.4935E+01  9.50
pu-240      4.6659E+01  4.6659E+01  4.6659E+01  4.6659E+01  4.6659E+01  4.6659E+01  4.66
pu-241      2.4857E+01  2.4856E+01  2.4856E+01  2.4854E+01  2.4848E+01  2.4832E+01  2.47
pu-242      1.2514E+01  1.2514E+01  1.2514E+01  1.2514E+01  1.2514E+01  1.2515E+01  1.25
am-241      9.5200E-01  9.5231E-01  9.5292E-01  9.5475E-01  9.6025E-01  9.7675E-01  1.02
am-243      2.3990E+00  2.3995E+00  2.4002E+00  2.4008E+00  2.4010E+00  2.4010E+00  2.40
cm-242      2.9934E-01  2.9937E-01  2.9941E-01  2.9925E-01  2.9771E-01  2.9156E-01  2.73
cm-244      9.0308E-01  9.0315E-01  9.0316E-01  9.0314E-01  9.0301E-01  9.0254E-01  9.01
cm-245      4.8234E-02  4.8234E-02  4.8234E-02  4.8234E-02  4.8234E-02  4.8234E-02  4.82
-----
totals      1.8163E+04  1.8163E+04  1.8163E+04  1.8163E+04  1.8163E+04  1.8163E+04  1.81
```


ORIGAMI results: radial Pu distribution

28.2	27.8	27.5	27.3	27.1	27.0	26.9	25.4	25.3	25.0	24.6	24.0	23.2	22.3
29.6	29.5	29.7	29.1	28.8	29.2	28.7	27.1	27.4	26.8	28.3	26.0	24.8	23.6
31.0	31.4	31.3	31.1	30.7	29.0	28.8	28.3	26.5	24.8				
32.1	32.2	32.8	32.5	32.8	32.5	31.5	29.6	30.3	30.2	29.3	28.7	27.2	25.8
33.2	33.4	34.0	34.2	33.4	32.4	30.1	30.9	30.7	29.7	28.1	26.7		
34.3	34.9	35.0	34.5	34.0	34.0	30.9	30.9	31.3	31.2	28.2	27.4		
35.1	35.2	35.7	34.9	34.4	34.9	31.8	31.0	30.9	30.9	30.7	29.3	27.9	
36.2	36.3	36.8	35.9	35.2	34.9	35.0	34.4	33.8	33.6	33.5	33.3	31.7	30.3
37.0	37.7	37.8	37.0	35.8	35.0	34.7	34.8	35.2	35.1	32.8	30.9		
37.7	38.0	38.7	38.8	37.3	35.9	35.5	38.3	36.0	34.8	32.9	31.4		
38.5	38.7	39.4	39.0	39.2	38.6	37.2	36.8	37.6	37.3	36.2	35.4	33.6	32.1
39.2	39.9	39.8	39.5	38.6	38.2	37.7	37.0	34.8	32.9				
39.7	39.8	40.2	39.4	39.1	39.3	38.4	38.2	38.5	37.5	36.9	36.6	35.0	33.6
40.3	40.0	39.7	39.4	39.1	38.8	38.5	38.6	38.3	37.8	37.2	36.5	35.5	34.6

Operator-provided pin-by-pin burnup (GWd/tU) map

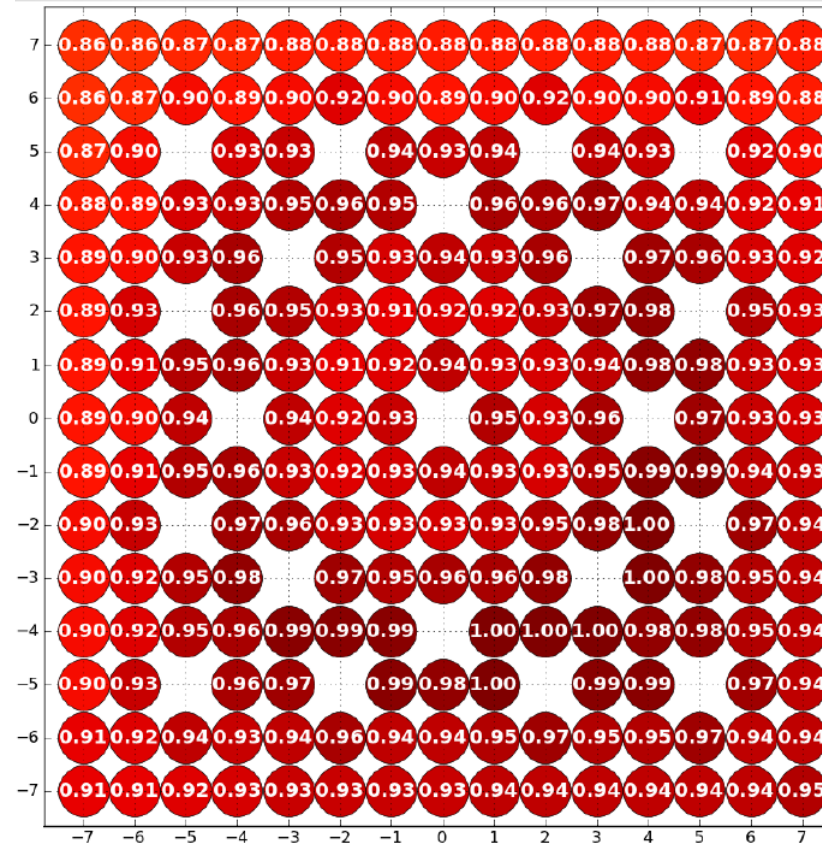


Pu content (g/MTU) in each Pin

ORIGAMI results: radial Cs-137 distribution

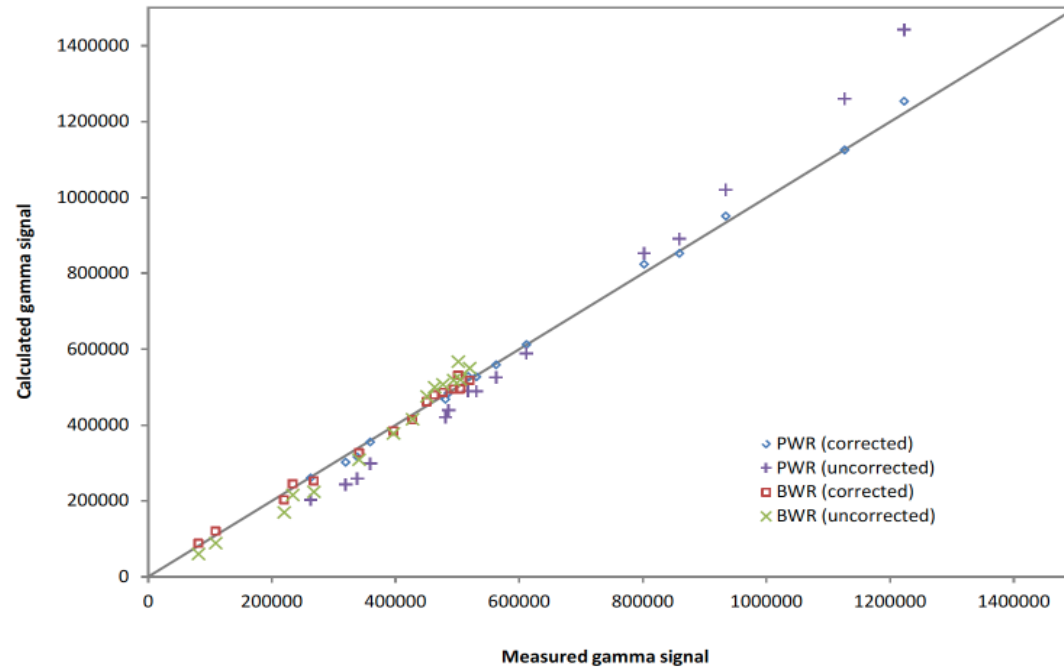
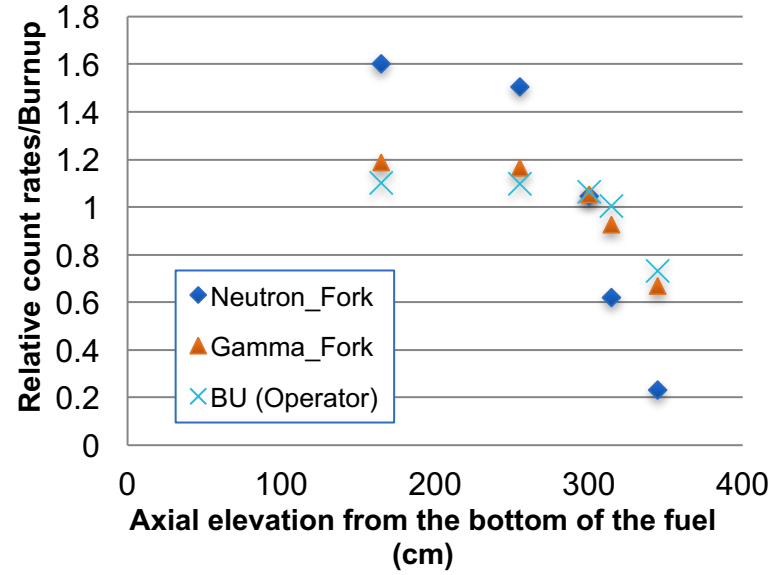
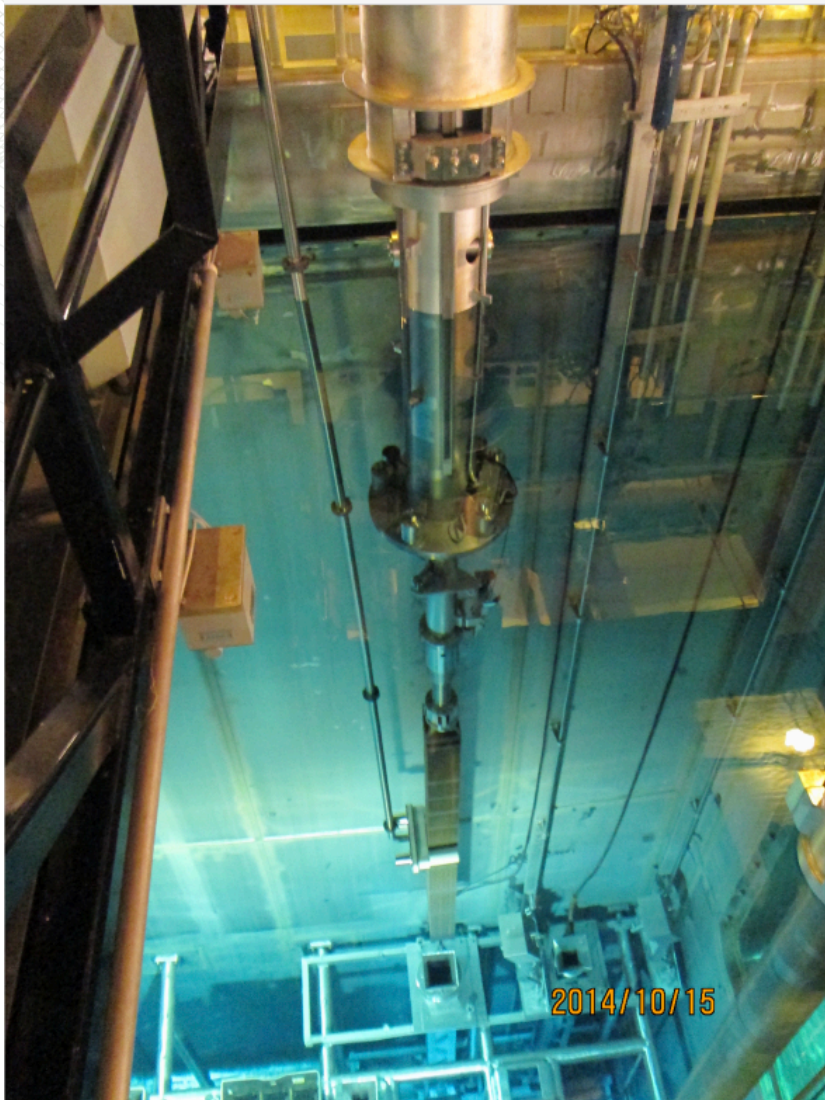
0.86	0.86	0.86	0.87	0.87	0.88	0.88	0.87	0.87	0.87	0.87	0.87	0.87	0.87	0.87
0.86	0.87	0.9	0.88	0.89	0.91	0.89	0.88	0.89	0.91	0.89	0.89	0.91	0.88	0.88
0.87	0.9		0.92	0.93		0.94	0.93	0.94		0.94	0.93		0.92	0.89
0.87	0.89	0.93	0.93	0.95	0.96	0.95		0.96	0.96	0.96	0.94	0.94	0.91	0.9
0.88	0.9	0.93	0.96		0.95	0.92	0.94	0.93	0.96		0.97	0.96	0.92	0.91
0.89	0.92		0.96	0.95	0.92	0.9	0.91	0.91	0.93	0.96	0.98		0.95	0.92
0.89	0.9	0.95	0.96	0.93	0.91	0.91	0.94	0.93	0.92	0.94	0.98	0.98	0.93	0.92
0.89	0.9	0.94		0.94	0.91	0.93		0.94	0.92	0.96		0.97	0.93	0.92
0.89	0.9	0.95	0.96	0.93	0.91	0.92	0.94	0.93	0.92	0.95	0.99	0.98	0.94	0.93
0.89	0.93		0.97	0.96	0.93	0.92	0.92	0.93	0.95	0.98	0.99		0.96	0.94
0.89	0.91	0.95	0.97		0.97	0.95	0.96	0.95	0.98		1	0.98	0.95	0.94
0.9	0.91	0.95	0.96	0.98	0.99	0.98		0.99	1	1	0.98	0.98	0.95	0.94
0.9	0.93		0.96	0.97		0.98	0.98	0.99		0.99	0.98		0.97	0.94
0.9	0.91	0.94	0.93	0.94	0.96	0.94	0.94	0.95	0.97	0.95	0.95	0.97	0.94	0.94
0.91	0.91	0.91	0.92	0.93	0.93	0.93	0.93	0.94	0.94	0.94	0.94	0.94	0.94	0.95

(a) Given burnup distribution (input)



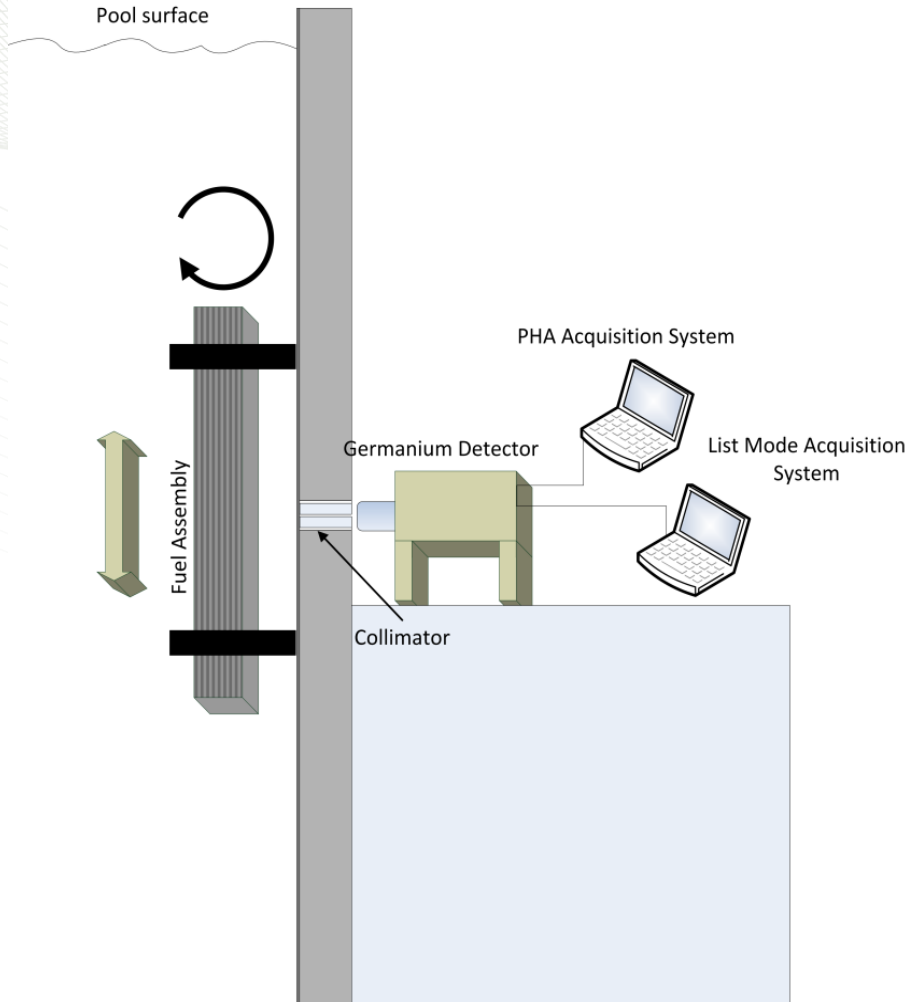
(b) Calculated Cs-137 distribution (output)

The Fork Measurements of the Swedish Fuel

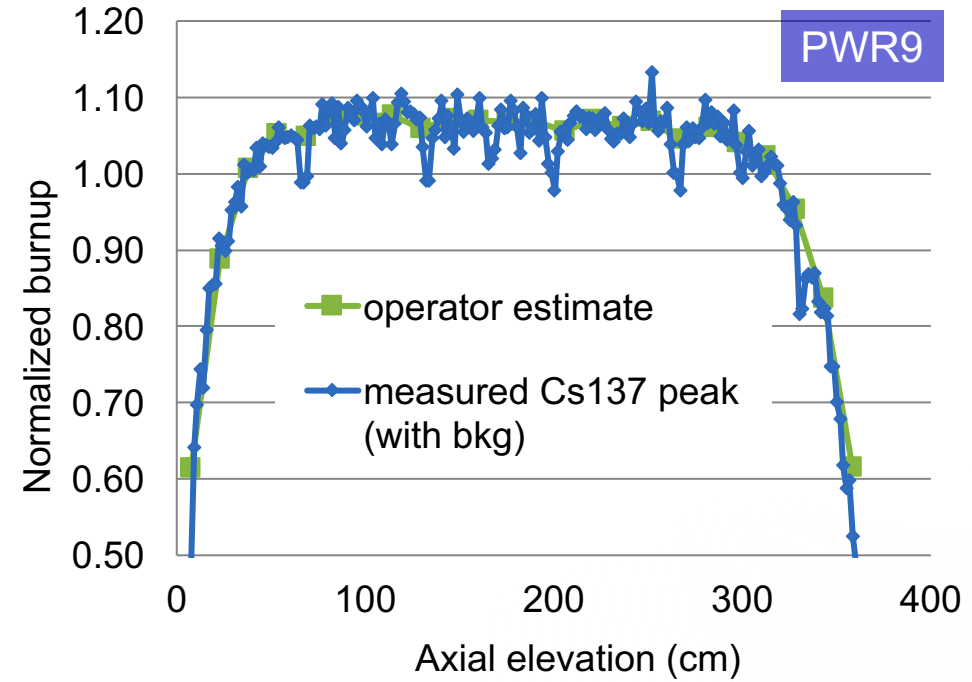


[1] I. Gauld, J. Hu, P. DeBaere, and et al., "In-Field Performance Testing of the Fork Detector for Quantitative Spent Fuel Verification," in *Proceedings of ESARDA*, Manchester, UK, ISBN 978-92-79-49495-6 (2015).

The Gamma Spectrum Measurements of the Swedish fuel



Scheme of the measurement set-up using high-purity Germanium detector [1]



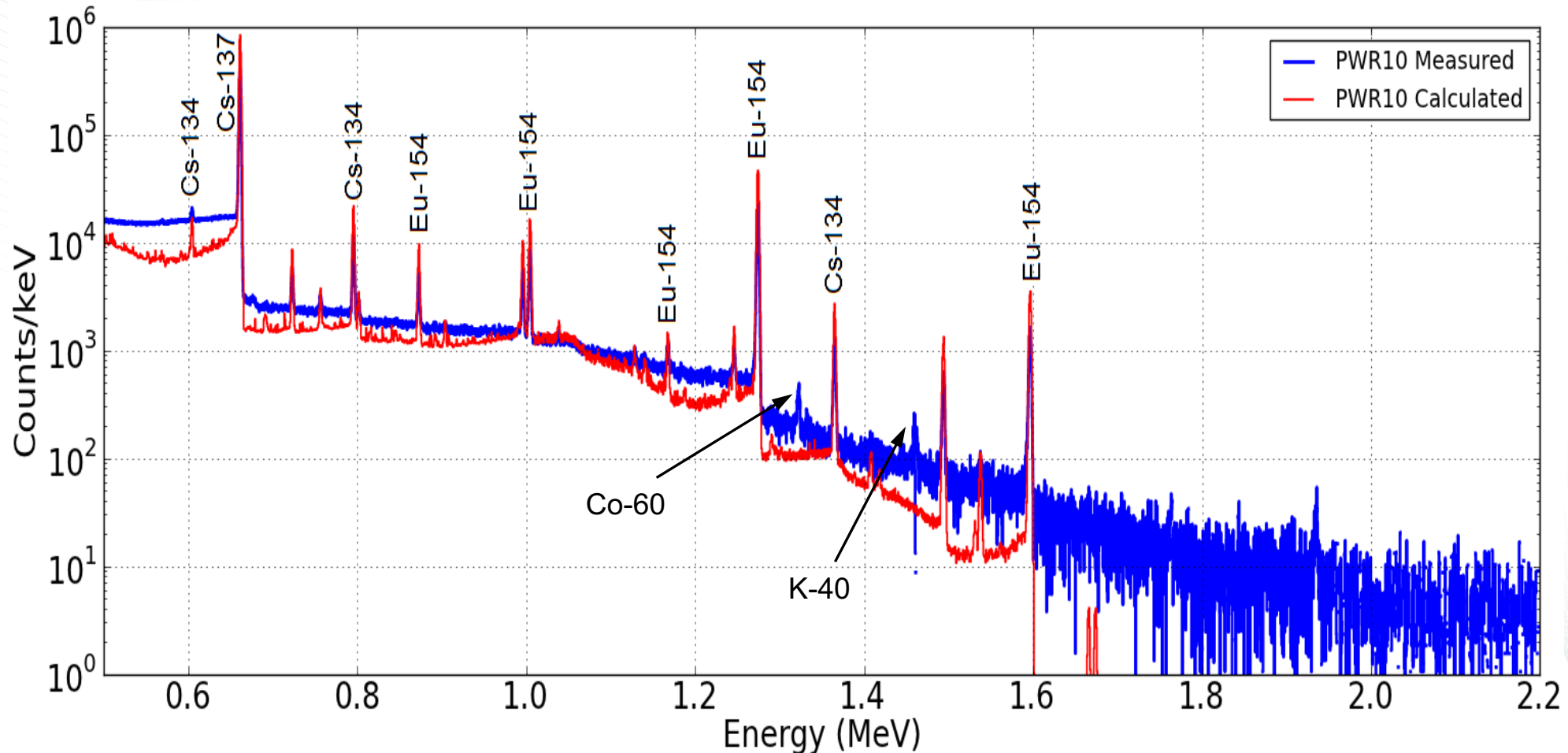
(a) Operator data vs. gamma scan

- The operator data on axial burnup distribution agrees well with axial gamma spectrometry scan (on PWR9).

[1] S. Vaccaro, et al., "PWR and BWR spent fuel assembly gamma spectra measurements," Nuclear Instruments and Methods (A), 833 (2016) 208-225.

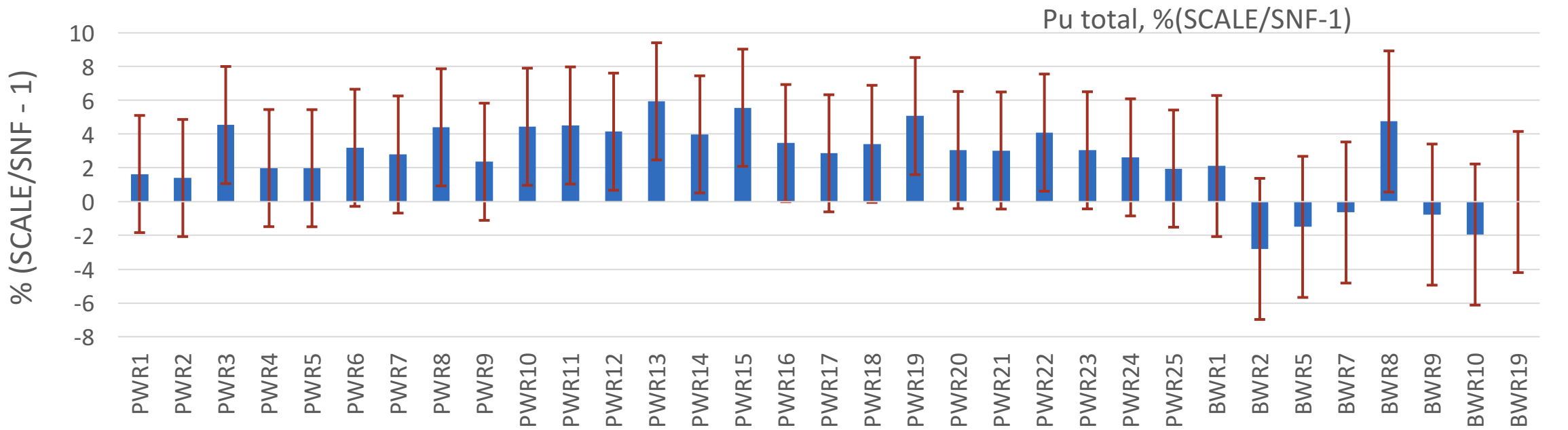
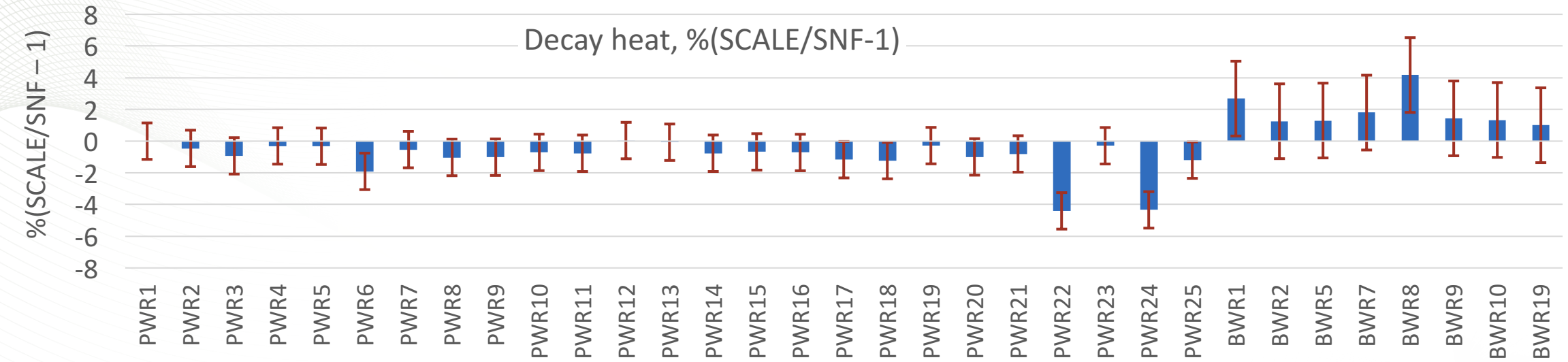
Comparison between Calculated and Measured Gamma Spectra

- Simulation of gamma spectra from Swedish spent fuel assemblies performed by LLNL
- ~1000 nuclides/node from ORIGEN
- Good agreement on the ratios among major gamma peaks



Calculated vs. measured gamma spectra of PWR10

Decay heat and Pu total: compared to CASMO/SIMULATE – SNF results



Summary

- Modeling and simulation is essential for advanced NDA testing for the Spent Fuel NDA project.
- SCALE/ORIGEN is a well-validated tool for spent fuel characterizations.
- ORIGAMI provides an efficient interface for fuel assembly burnup calculations using detailed operator/measured data. Now publicly available in SCALE 6.2.
- Well-characterized nuclide compositions/source terms have been generated for the SKB fuels. These results will be used to assess instrument performance.
- Calculations have been compared to measured gamma spectra, and to results from an industry code. Good agreements have been observed.
- More details about decay heat uncertainty analysis will be presented separately.

Acknowledgement

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- The authors would also like to thank Steven Skutnik (UTK), Mark Williams, and Will Wieselquist for help on ORIGAMI customization; Germina Ilas for processing the SKB fuel design and operator data.

Questions?

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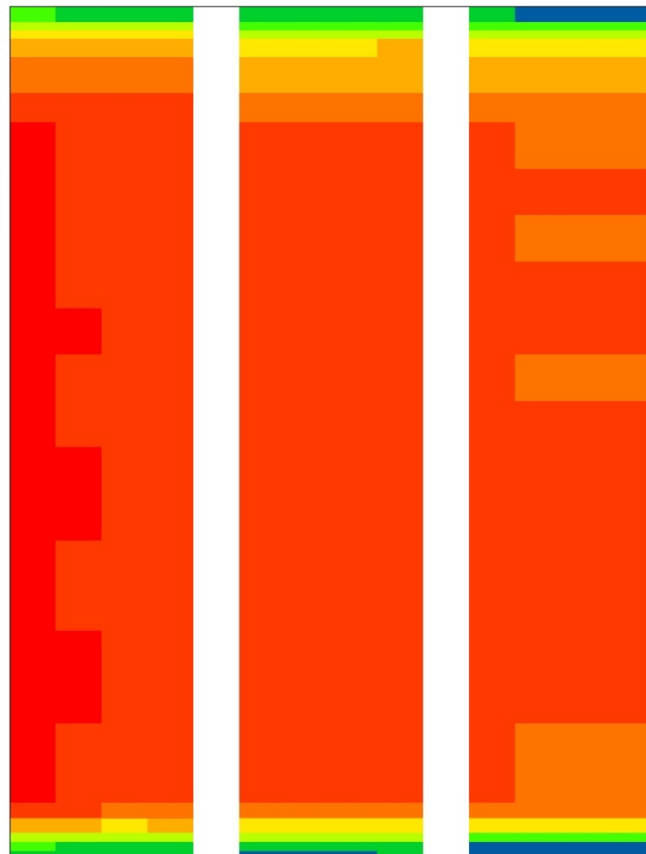
Backup slides

Accuracy of SCALE/ORIGEN: nuclides

Isotope	Number of measurements	SCALE 6.1 ENDF/B-VII		Application
		$(C/E-1)_{avg}$ (%)	σ (%)	
²³⁴ U	55	12.4	17.6	Nuclear Safeguards
²³⁵ U	92	1.2	3.5	
²³⁶ U	77	-1.9	3.5	
²³⁸ U	92	-0.1	0.4	
²³⁸ Pu	77	-11.7	5.9	
²³⁹ Pu	92	4.1	3.5	
²⁴⁰ Pu	92	2.2	3.4	
²⁴¹ Pu	92	-1.4	4.5	
²⁴² Pu	91	-5.9	6.1	
²⁴¹ Am	39	10.2	20.7	
²⁴⁴ Cm	57	-4.4	11.1	Main neutron emitter
¹⁰⁶ Ru	31	7.9	22.7	Gamma emitter
¹⁰³ Rh	8	9.1	10.9	Gamma emitter
¹³⁴ Cs	59	-7	7.1	Gamma emitter
¹³⁷ Cs	73	-0.7	3.1	
¹⁴⁸ Nd	77	0.6	1.4	burnup indicator used by DA
¹⁴⁴ Ce	32	-2.1	8.1	Gamma emitter
¹⁴⁹ Sm	20	1.9	6.2	Neutron absorber
¹⁵¹ Sm	24	-2.1	4.4	
¹⁵⁴ Eu	44	4.2	10.4	Gamma emitter
¹⁵⁵ Gd	19	-8.4	14.4	Neutron absorber

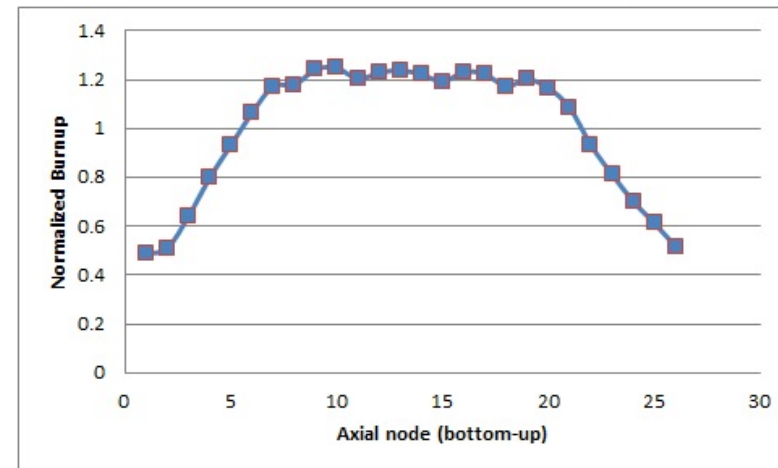
Note: these results were based on PWR DA data on small spent fuel samples (of fuel pellet size). Accuracies on assembly average are expected to be better because average operating conditions are better known than that of a small region.

ORIGAMI results: axial Pu distribution



The generated “3D” nuclide compositions can also be useful for shielding and criticality safety analysis.

XZ cross-sectional view of Pu content
(the cut plane goes through 2 guide tubes)



Axial burnup profile (derived from Cs-137 scans)