Validation of Historic SNM Isotopic Calculations

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Overview

- Motivation for reviewing historic data
- Current isotopic methodology
- Validation methodology
- Results
- Submission of corrections to NMMSS
- Conclusion

Motivation for Reviewing Data

- Internal Review of SNM Inventory of Record.
  - Complete QA validation of all data used in safety-related or regulatory reporting applications.
  - "Complete and accurate."
  - Multiple database transitions over history of sites.
  - Multiple methodology transitions over history of sites.
- Draft ANSI N15.8
  - "Refinement of the element and isotopic computations…should be considered as new technologies evolve."

Current Isotopic Methodology

- Depends on what site one is talking about.
  - Oconee (B&W 15x15 PWR)
    - Batch-average CASMO-3 (2D transport code) model.
    - Calculates [sub]batch-average isotopic number densities over range of burnups.
    - Interpolate on assembly burnup.
  - McGuire and Catawba (Westinghouse 17x17 PWRs)
    - Duke-internal utility codes (ISOTAB/BURN).
    - Calculates multi-variable dependent isotopics per kgU.
    - Interpolates on enrichment and assembly burnup.

ANSI	Period	Total U	U-235	U-236	U-238	Total Pu	Total Pu Fissile	Pu-239	Pu-240	Pu-241	Pu-242	Burnup
NJ05K7	INITIAL	454990	17078	0	437912	0	0	0	0	0	0	0
NJ05K7	BOC	454856	17062.2	0	437793	0	0	0	0	0	0	0
NJ05K7	BURNUP	452404	15307.2	335.17	436761	794.76	748.81	740.42	45.66	8.39	0.29	3442.58
NJ05K7	BURNUP	448241	12561	850.25	434830	1990.93	1748.12	1655.96	236.45	92.16	6.36	9731.77
NJ05K7	BURNUP	445481	10901.7	1145.9	433433	2642.35	2232.25	2045.19	390.29	187.06	19.81	14150.8
NJ05K7	EOC	443427	9751.8	1346.54	432329	3072.16	2525.38	2254.94	509.75	270.44	37.03	17565.1
NJ05K7	BURNUP	443316	9687.9	1356.91	432271	3091.04	2536.79	2262.1	516.06	274.69	38.19	17759
NJ05K7	BURNUP	442832	9428.93	1400.03	432003	3180.63	2594.09	2299.32	543.2	294.77	43.34	18580.5
NJ05K7	BURNUP	442148	9068.87	1460.23	431619	3305.72	2672.5	2348.73	581.88	323.77	51.34	19747.2
NJ05K7	BURNUP	441616	8791.49	1507.17	431317	3403.7	2732.78	2385.7	612.7	347.08	58.22	20664
NJ05K7	EOC	440225	8086.1	1622.87	430516	3639.84	2871.51	2465.39	690.56	406.12	77.77	23080.4
NJ05K7	BOC	440236	8074.88	1622.41	430539	3622.51	2856.14	2454.83	688.67	401.31	77.7	23080.4
NJ05K7	BURNUP	438741	7352.09	1735.37	429654	3846.48	2977.82	2517.51	767.53	460.31	101.13	25714.8
NJ05K7	BURNUP	436735	6443.67	1876.86	428414	4135.92	3124.03	2585.15	872.74	538.88	139.15	29308.6
NJ05K7	BURNUP	432945	4933.68	2087.14	425924	4583.28	3310.42	2649.83	1047.86	660.59	225	36233.4
NJ05K7	EOC	431419	4398.53	2151.49	424869	4728.12	3356.68	2657.98	1108.56	698.7	262.88	39061.4
NJ05K8	INITIAL	454245	17057	0	437188	0	0	0	0	0	0	0
NJ05K8	BOC	454112	17034.3	0	437077	0	0	0	0	0	0	0
NJ05K8	BURNUP	451712	15315	328.44	436068	778.89	734.79	726.92	43.83	7.87	0.27	3372.85
NJ05K8	BURNUP	447377	12459.2	863.15	434055	2019.41	1769.76	1673.85	242.87	95.91	6.78	9937.49
NJ05K8	BURNUP	444467	10720.5	1173.09	432573	2701.11	2272.66	2074.47	406.57	198.19	21.88	14621.6
NJ05K8	EOC	442336	9541.16	1376.78	431418	3134.38	2563.97	2278.68	529.51	285.29	40.9	18187.1
NJ05K8	BURNUP	442109	9416.1	1397.21	431296	3174.02	2588.34	2293.9	542.25	294.44	43.43	18580.8
NJ05K8	BURNUP	441142	8908.74	1482.09	430751	3350.44	2698.09	2362.29	597.21	335.8	55.14	20239.4
NJ05K8	BURNUP	439813	8231.67	1594.21	429987	3580.72	2834.63	2441.78	672.41	392.85	73.68	22548.4
NJ05K8	BURNUP	438802	7734.78	1672.78	429394	3737.04	2921.55	2487.84	726.53	433.71	88.96	24325
NJ05K8	EOC	436266	6564.84	1855.24	427846	4106.17	3111.52	2577.61	859.8	533.91	134.85	28856.6
NJ05K8	BOC	436275	6552.3	1854.78	427868	4089.65	3097.57	2569.77	857.63	527.8	134.45	28856.6

Isotopic Validation Methodology

- Variant of "Oconee method."
  - CASMO-3 core depletions.
    - Average core conditions.
    - RCS boron concentration important factor.
      - Significant impact on U consumption/Pu production.
      - At low BU, model with higher BOC concentration, then transition to cycle average concentration.
    - Average BP enrichment and pull ~20 GWd/MTU.
      - Also impacts U/Pu characteristics.
    - Calculate for range of assembly average enrichments for each fuel assembly design (2.00, 2.50, … , 5.00).
    - Calculate over large, discrete range of burnups.

Validation Methodology (cont'd)

- Selection of fuel characteristics.
  - Six different fuel designs used at McGuire/Catawba, no fewer than fifteen distinct designs at Oconee.
  - Must consolidate in order to make validation of entire SNM inventory feasible.
  - Consider "neutronic similarities" of varying fuel designs.
    - Ex: Westinghouse "STD" fuel essentially identical to "RFA."
    - Selection of "intermediate" B&W fuel designs at Oconee to bound entire inventory.
  - For McGuire/Catawba, collapse six to four.
  - For Oconee, collapse over fifteen to one.
- Interpolate calculated number densities as a function of enrichment and burnup.
- Derive calculated isotopics based on interpolated number densities.

Validation Methodology (cont'd)

- Validation of final (discharge) assembly burnups.
  - All methods for calculating isotopics dependent upon burnup of assembly.
  - If the burnup is wrong, the isotopics are wrong.
- Compare "measured" burnups in SNM database to predicted values in core design calculations.
- Identify any discrepancies, replace burnups, and correct isotopics accordingly.

Validation Methodology (cont'd)

Parameter	mbf	W-OFA	MkBW	W-RFA	Adv-MkBW
Fuel Temperature (TFU)	811 K	949.8 K			
Moderator Temperature (TMO)	577 K	584.3 K			
Inter-assembly Pitch (CHW)	21.81 cm	21.504 cm			
Reactor Pressure (PRE)	151.7 bar	155 bar			
Boron Concentration (BOR)	1400/700 ppm	1400/600 ppm			600 ppm
Average Power Density (PDE)	31.29 W/gU	41.73 W/gU	38.74 W/gU	38.10 W/gU	38.5 W/gU
Burnup Intervals (GWd/MTU)	0, 0.2, 0.4, 0.5, 1, 3, 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60				0, 8, 9, 14, 15, 20, 25, 30
Enrichment Intervals (wt.% U-235)	2.00, 2.50, … , 5.00				*

Validation Methodology (cont'd)

For U-235 and U-236:

$$M_{iso}(E_i) = \left[\frac{N_{iso}(E_i) \times AW_{iso}}{N_{U-235}(E_0) \times AW_{U-235}}\right] \times M_{U-235}(E_0) \qquad \text{Equation (1)}$$

For U-238, Pu-239, Pu-240, Pu-241, and Pu-242:

$$M_{iso}(E_i) = \left[\frac{N_{iso}(E_i) \times AW_{iso}}{N_{U-238}(E_0) \times AW_{U-238}}\right] \times M_{U-238}(E_0) \qquad \text{Equation (2)}$$

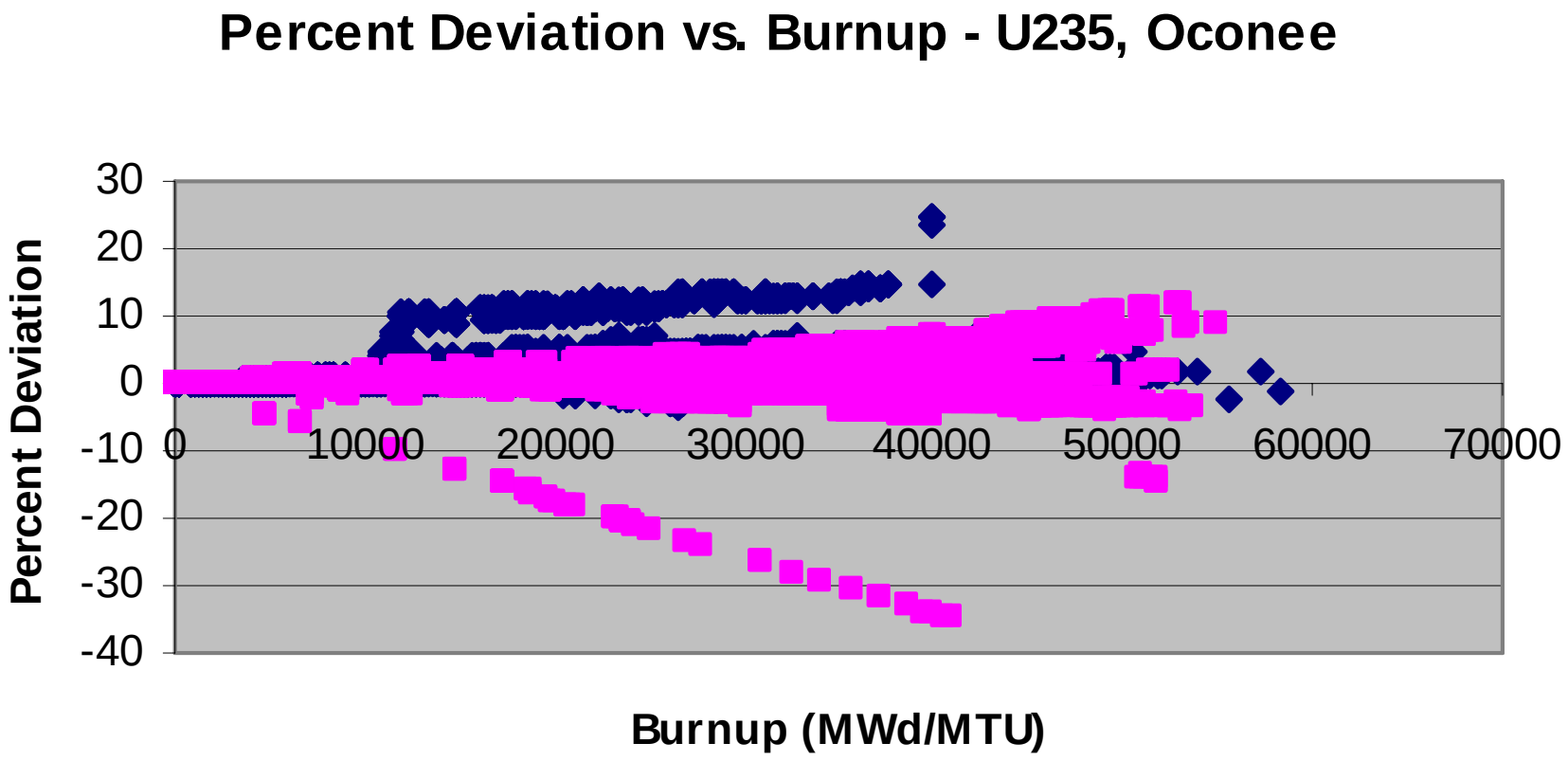
Where:

$M_{iso}(E_i)$ = isotopic mass at the specified burnup (E_i),
$N_{iso}(E_i)$ = isotopic number density at the specified burnup (E_i),
AW_{iso} = atomic weight of the desired isotope,
$N_{U-235}(E_0)$ = initial (zero burnup) U-235 number density,
$N_{U-238}(E_0)$ = initial (zero burnup) U-238 number density,
AW_{U-235} = atomic weight of U-235,
AW_{U-238} = atomic weight of U-238,
$M_{U-235}(E_0)$ = initial (zero burnup) U-235 mass,
$M_{U-238}(E_0)$ = initial (zero burnup) U-238 mass.

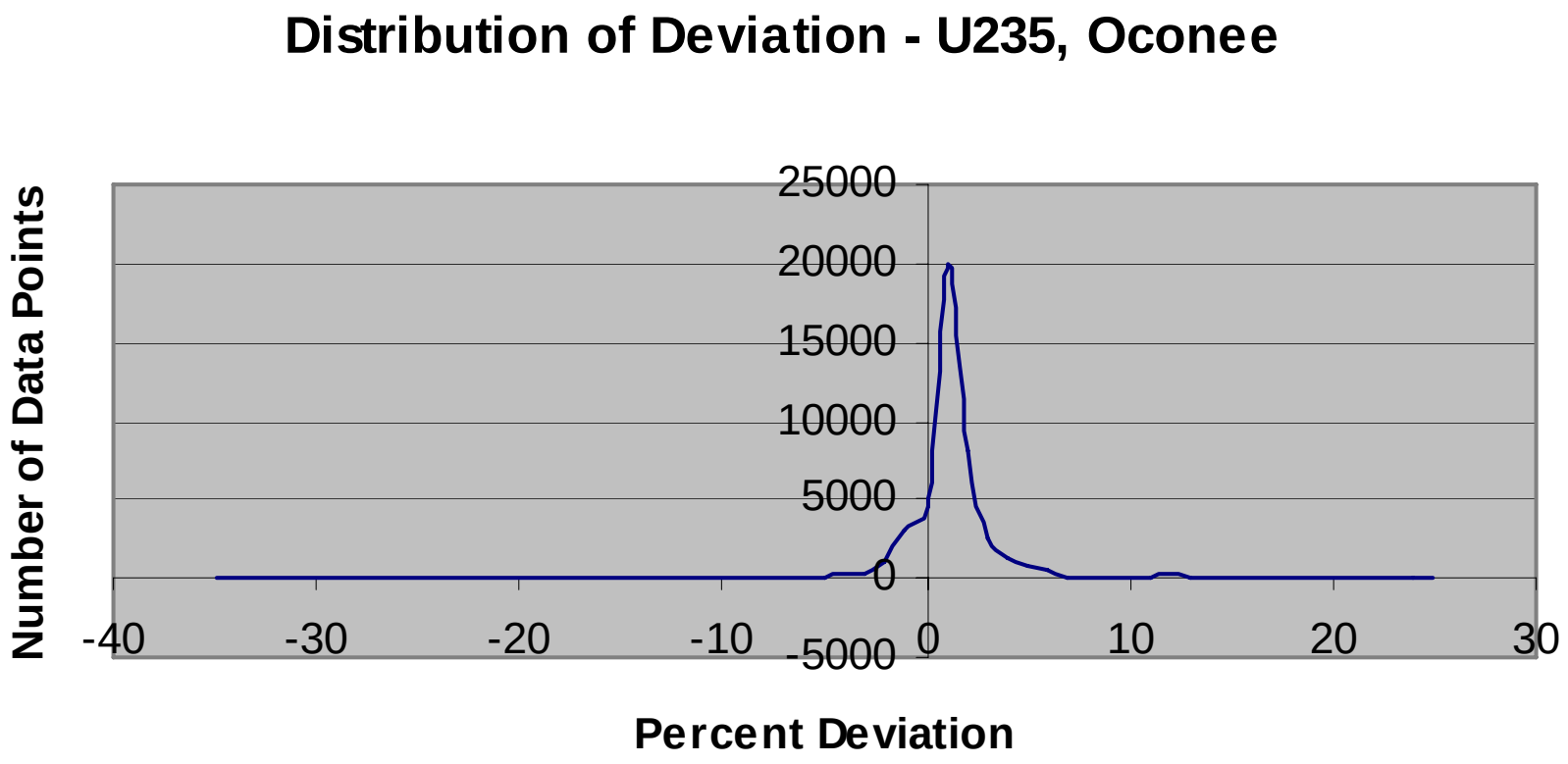
Validation Acceptance Criteria

- Comparison of calculated estimates to "actual" isotopics in inventory of record.
- Two acceptance criteria:
  - Statistically-normal distribution of deviation (bell curve) for entire sample of given fuel design.
  - Absolute percentage difference of no more than 10% for individual assemblies.
- Some assemblies "on the line" can be statistically excluded if 95/95 integrity of data set is preserved.

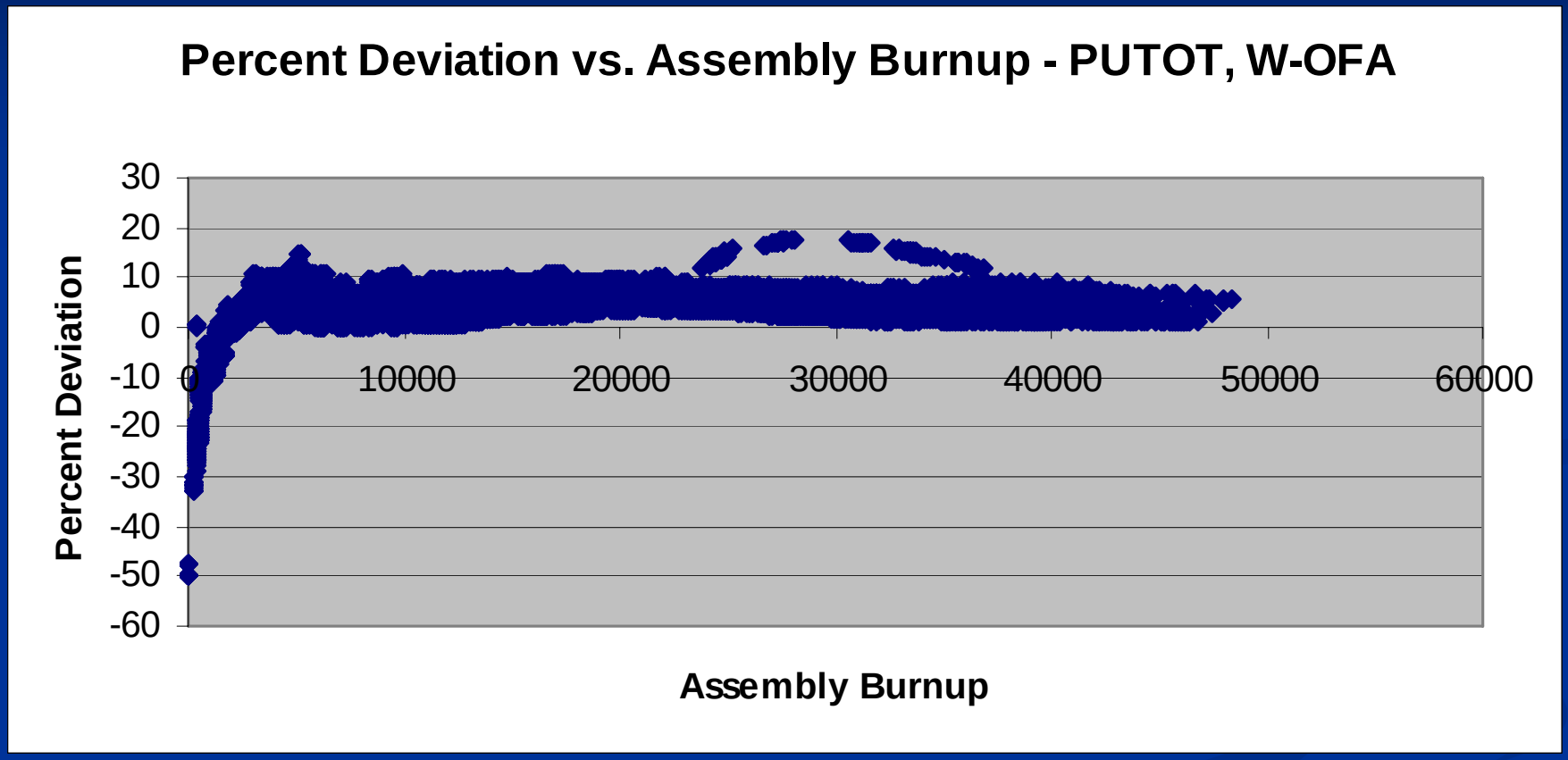
Validation Results (Oconee)



Validation Results (Oconee)



Validation Results (W-OFA)



Validation Results Summary

- In total, eight "groups" of assemblies were identified as having discrepant isotopic data.
  - Four of the eight groups date to the 70's and early 80's.
  - One group consists of lead test assemblies.
  - Two consist of an oddball mix of blanketed and non-blanketed fuel.
  - One consists of a small set of assemblies (four) that exclusively exceeded 50 GWd/MTU burnup.
- See any trends?

Ancient and/or off-normal batches of fuel are most susceptible to errant isotopic data.

WHAT A SURPRISE!!!!

Submitting Corrections to NMMSS

- Action code "M" (on-site gains/losses) Form 741 submitted to NMMSS.
- Change Type Code 34 "Receipts – Miscellaneous" for positive adjustments.
- Change Type Code 54 "Shipments – Miscellaneous" for negative adjustments.
- Concise Note included to explain reason for making adjustments.
  - "RECALCULATION OF ISOTOPIC DATA DURING QA OF SNM DATABASE"

DOE/NRC Form 741 for XFV

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XFV XFV     58 A M103                                                  11152007  X
XFV XFV     58 A M201540310-MISC                      10309  J
XFV XFV     58 A M501540310-MISC                 133200       6757        900
XFV XFV     58 A M202340320-MISC                      20309  J
XFV XFV     58 A M502340320-MISC              133725100       7843    1049600
XFV XFV     58 A M203340350-MISC                      50309  J
XFV XFV     58 A M503340350-MISC                 154900     680197     147100
XFV XFV     58 A M6WHOLE REPORT    01 RECALCULATION OF ISOTOPIC DATA DURING
XFV XFV     58 A M6SHOLE REPORT    02 QA OF SNM DATABASE
XFV XFV     58 A M70110       -100           92
XFV XFV     58 A M70220     -47100      -100032
XFV XFV     58 A M70350        600           32
XFV XFV     58 A M70450      21000           92
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Conclusion

- Performing a full validation of historic SNM isotopics is feasible using a relatively simple method.
- Multiple fuel assembly designs can be collapsed into a few "similar" designs for comparison's sake.
- Oddball fuel batches (LTAs, split batches) and older data are most likely to be wrong.
- Submitting fixes to NMMSS for stuff like this is relatively painless and makes you sleep better at night.

Questions?