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Validation and uncertainties for GU3: the PSI experience

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Summary

- Method
- Validation
- Uncertainties

- All results available here:

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Analysis for the ARIANE GU3 sample: nuclide inventory and decay heat

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Motivation and method

- GU3 is part of the ARIANE program, and was irradiated in Gösgen, Switzerland
- Part of the CASMO5 validation with PIE set at PSI (PROTEUS, ARIANE, MALIBU): 27 samples
- UO_2 sample, 4.1% enr., in 15x15 PWR assembly, 3 consecutive cycles (16,17,18), in 2 assemblies
- Access to the detailed irradiation histories for both assemblies from core follow-up validation with CASMO5/SIMULATE-3

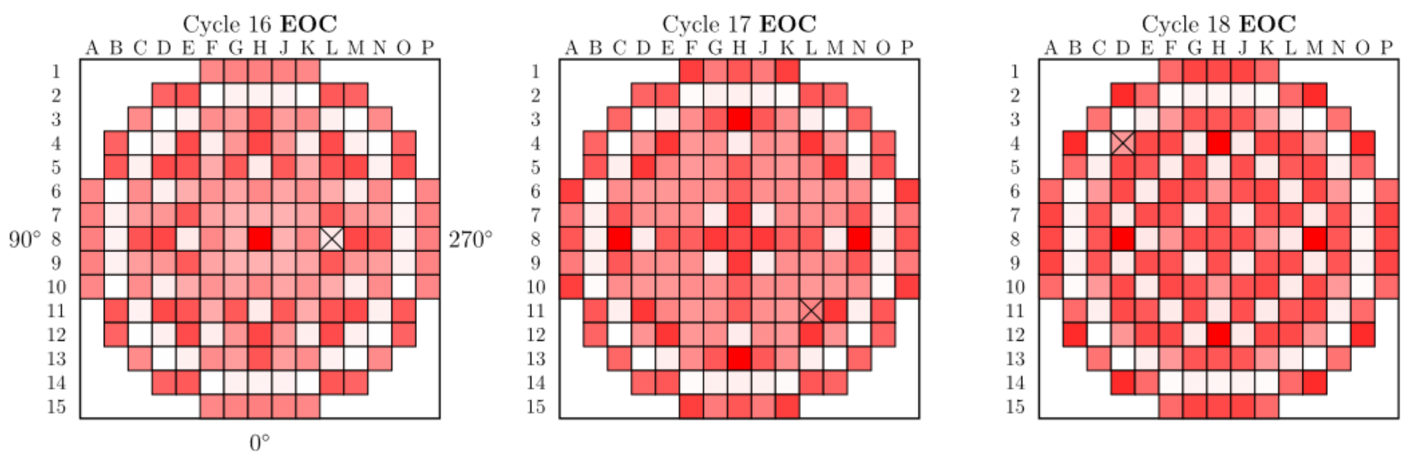
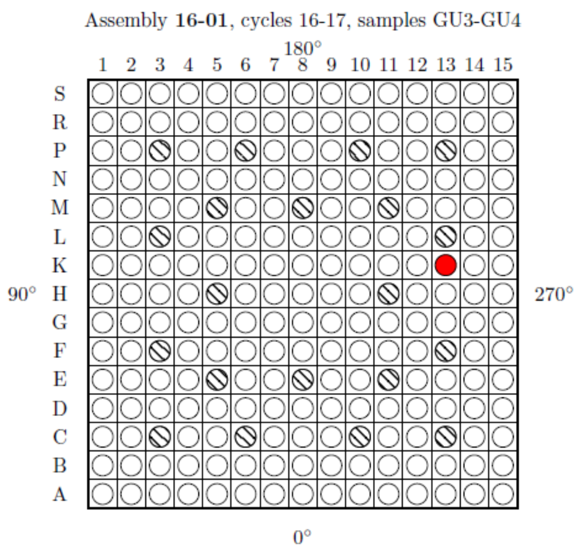


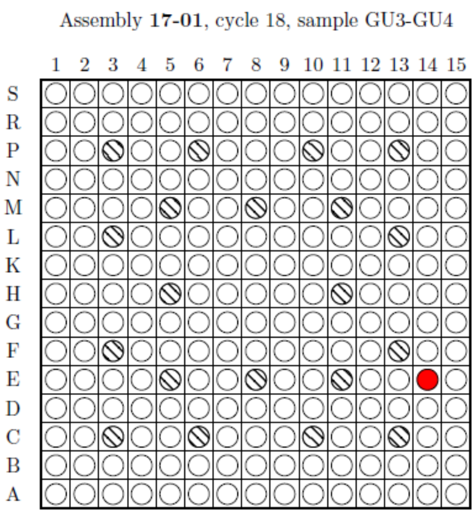
Fig. 2. Locations of the assemblies 16-01 (cycles 16 and 17) and 17-01 (cycle 18) containing the GU3 sample. The positions of both assemblies are indicated by a cross. The colors are proportional to the assembly burnup obtained from SIMULATE-3 at the end of each cycle (EOC).

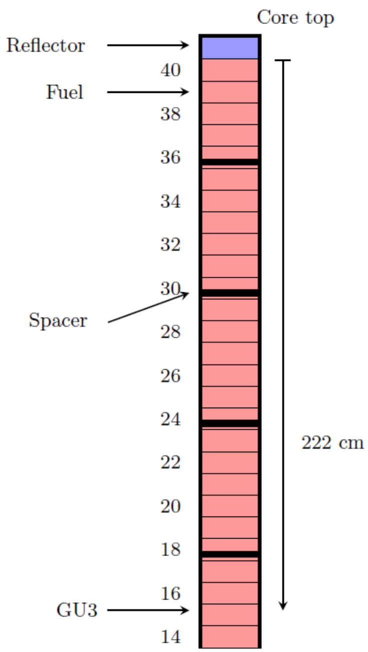
Motivation and method

- GU3 was analyzed in ITU and GU3' in SCK (same sample)

- Different measured nuclide concentrations, different measurement times.
  - Nd148 differs by 5%
  - Some ITU measurements were rejected by ARIANE
  - FIMA differs by 5%
  - Recommendations by ORNL (used in SG10)







Tools

- CASMO5: different versions, different nuclear data libraries
- Irradiation history based on detailed information from SIMULATE-3
  - 20 steps/cycle
  - Changing moderator and fuel temperatures, power density, reactor pressure, and eventually the control rod position.
  - No burnup adjustment was necessary to match the Nd-148 from GU3'
- Estimated sample burnup: 52.5 ± 0.5 MWd/kg (U).

Table 2. Comparison of average C/E-1 (in%) between different types of calculations for GU3 and GU3', see text for details.

Code	Library	case	GU3' (SCK) 52 isotopes AC/FP	GU3' (SCK) 45 isotopes AC/FP	GU3 (ITU) 45 isotopes AC/FP	Reference [8] 50 isotopes AC/FP
CASMO5 2.03	ENDF/B-VII.1	1	−2/+3	+1/+2	−1/+1	+2/+1
CASMO5 2.13	ENDF/B-VII.1	2	−3/+1	+0/+1	−2/+0	+1/-0
CASMO5 2.12, 2.13	ENDF/B-VII.1	3,4	−2/+1	+0/+1	−2/+0	+1/+3
CASMO5 3.01, 3.02	ENDF/B-VII.1	5,11	−3/+1	+0/+1	−2/+0	+1/+3
CASMO5 3.01, 3.02	ENDF/B-VIII.0	6,12	−3/+1	−0/+0	−3/+0	
CASMO5 3.01	JEFF-3.1.1	7	−10/+5	−4/+2	−6/+1	−2/+6
CASMO5 3.01, 3.02	JEFF-3.2	8,9	−3/+1	−1/+1	−4/+0	−0/+3
CASMO5 3.02	JENDL-4.0	10	−2/+2	+1/+2	−2/+1	+2/+4
SCALE [18]	SCALE-6		−1/+2			
WIMS [22]	JEFF-3.1		−1/+8		−4/−1	
VESTA [23]	ENDF/B-VII.0		−1/−2		−5/+13	
VESTA [23]	ENDF/B-VII.1		+0/−4		−5/+11	
VESTA [23]	ENDF/B-VIII.0		+0/−2		−5/+14	
VESTA [23]	JEFF-3.1		−2/+0		−6/+13	
VESTA [23]	JEFF-3.2		+0/+0		−6/+14	
VESTA [23]	JEFF-3.3		+1/−1		−5/+14	
TRITON [8]	SCALE-5.1					+1/+6

Uncertainties due to nuclear data

- Sampling approach (TMC like): repeating 300 times the same calculations, each time with sampled nuclear data using
  - ENDF/B-VIII.0, JEFF-3.3 and JENDL-4.0 covariance files (separately for each library)
  - Partial variation for XS and FY

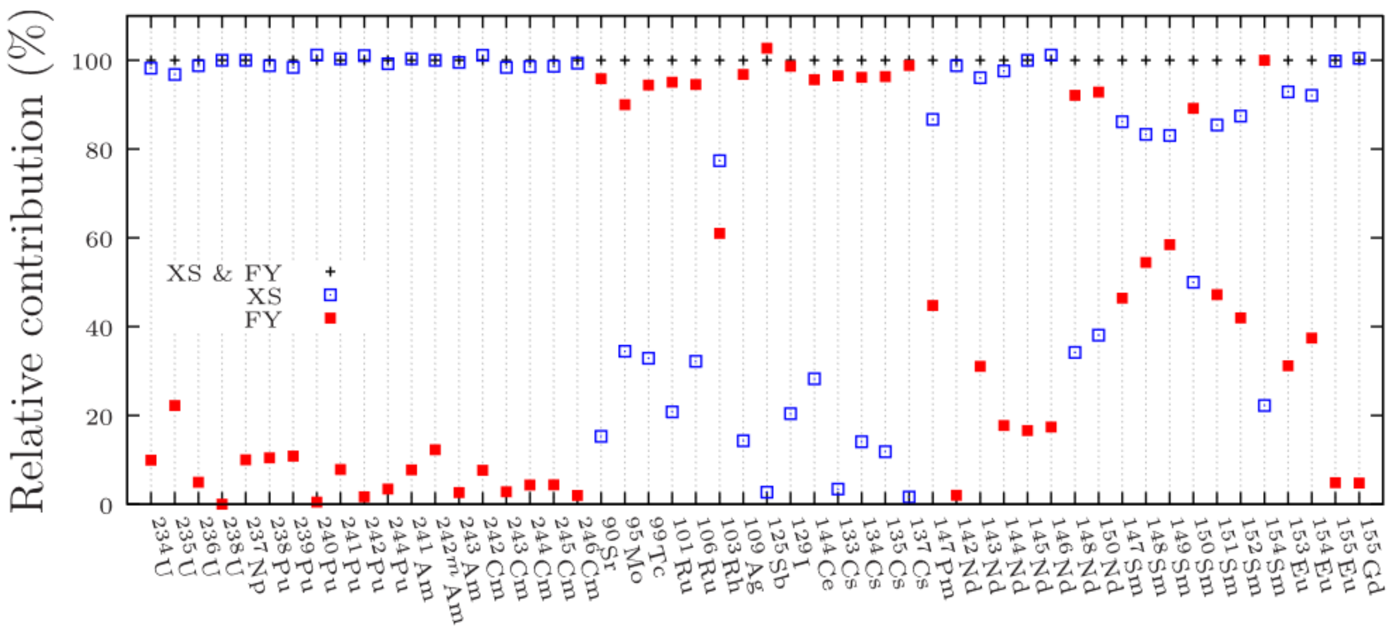


Fig. 5. Relative contributions of the cross sections (called XS) and fission yields (called FY) to the total uncertainties based on the ENDF/B-VIII.0 covariance library.

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Uncertainties due to nuclear data

	ENDF/B-VIII.0 GU3'	JEFF-3.3 GU3'	JENDL-4.0 GU3'
^{234}U	2.3	2.2	7.9
^{235}U	1.2	1.6	1.8
^{236}U	0.8	1.7	1.2
^{238}U	0.0	0.0	0.0
^{237}Np	3.3	3.9	4.0
^{238}Pu	4.8	9.4	7.0
^{239}Pu	1.8	1.7	2.2
^{240}Pu	4.3	2.5	4.4
^{241}Pu	3.2	3.1	3.4
^{242}Pu	4.8	8.5	8.6
^{244}Pu	8.9	8.1	9.2
^{241}Am	3.4	3.1	3.9
^{242m}Am	3.8	3.2	4.5
^{243}Am	8.5	7.7	9.0
^{242}Cm	3.6	2.7	4.1
^{243}Cm	11	16	12
^{244}Cm	9.7	9.3	10
^{245}Cm	15	14	15
^{246}Cm	24	21	24

	ENDF/B-VIII.0 GU3'	JEFF-3.3 GU3'	JENDL-4.0 GU3'
^{90}Sr	0.7	1.4	0.7
^{95}Mo	0.9	0.7	0.9
^{99}Tc	1.4	0.8	1.6
^{101}Ru	2.8	0.9	3.1
^{106}Ru	1.5	1.7	1.5
^{103}Rh	1.7	1.7	1.3
^{109}Ag	21	4.4	20
^{125}Sb	18	27	30
^{129}I	3.0	6.1	3.5
^{133}Cs	28	2.3	30
^{134}Cs	29	4.6	30
^{135}Cs	7.1	20	7.6
^{137}Cs	6.7	3.6	6.9
^{144}Ce	0.4	0.6	0.5
^{147}Pm	2.5	1.2	1.3
^{142}Nd	5.1	5.0	0.8
^{143}Nd	2.0	3.6	0.9
^{144}Nd	1.2	2.2	0.4
^{145}Nd	2.0	0.9	0.4
^{146}Nd	1.7	0.7	0.3
^{148}Nd	0.4	0.6	0.4
^{150}Nd	0.4	0.9	0.5
^{147}Sm	2.2	1.2	1.2
^{148}Sm	1.8	1.9	1.0
^{149}Sm	1.7	3.5	1.6
^{150}Sm	1.2	1.3	1.0
^{151}Sm	2.7	12	2.0
^{152}Sm	2.6	3.8	1.2
^{154}Sm	1.6	7.3	1.7
^{153}Eu	3.3	2.1	1.1
^{154}Eu	2.8	2.3	1.3
^{155}Eu	24	24	1.1
^{155}Gd	23	23	1.1

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Uncertainties due to other quantities

- Operating conditions:
  – Fuel & moderator temperatures, boron concentration (uniform, 2 %)
  – Burnup (uniform, 0.25%, certainly underestimated, given recent results)
- Manufacturing tolerances:
  – Radii of the fuel and guide tubes, positions, pitch (uniform, 0.5%, with constrains)
  – Fuel density and enrichment (uniform, 0.5%)

	ND min−max	TFU	TMO	BOR	RAD	ENR +DEN	(X-Y)	DEP	PITCH
^{234}U	2.3−7.9	0.0	0.3	0.0	0.1	0.1	0.2	0.2	0.5
^{235}U	1.2−1.8	0.2	1.8	0.0	0.6	0.6	1.0	0.4	1.1
^{236}U	0.8−1.7	0.0	0.3	0.0	0.0	0.2	0.1	0.1	0.1
^{238}U	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
^{237}Np	3.3−4.0	0.1	0.9	0.0	0.2	0.3	0.2	0.2	1.1
^{238}Pu	4.8−9.4	0.0	1.8	0.0	0.2	0.4	0.4	0.4	2.0
^{239}Pu	1.7−2.2	0.2	1.6	0.0	0.2	0.1	0.4	0.0	1.6
^{240}Pu	2.5−4.4	0.1	1.0	0.0	0.1	0.1	0.2	0.1	0.6
^{241}Pu	3.1−3.4	0.2	1.8	0.0	0.2	0.3	0.2	0.1	1.5
^{242}Pu	4.8−8.6	0.1	1.0	0.0	0.5	0.7	0.6	0.4	0.9
^{244}Pu	8.1−9.2	0.1	1.8	0.0	0.7	0.9	1.1	0.7	1.9
^{241}Am	3.1−3.9	0.2	1.8	0.0	0.2	0.3	0.3	0.1	2.7
^{242m}Am	3.2−4.5	0.3	3.2	0.1	0.4	0.3	0.7	0.2	3.6
^{243}Am	7.7−9.0	0.1	1.3	0.0	0.6	0.7	0.7	0.5	1.7
^{242}Cm	2.7−4.1	0.1	1.8	0.0	0.3	0.5	0.2	0.3	1.6
^{243}Cm	11−16	0.1	2.6	0.1	0.3	0.6	0.3	0.5	2.7
^{244}Cm	9.3−10	0.1	2.4	0.1	0.6	0.9	1.0	0.8	3.1
^{245}Cm	14−15	0.1	4.9	0.1	0.5	0.9	1.1	0.9	4.8
^{246}Cm	21−24	0.1	2.9	0.1	0.9	1.2	1.6	1.2	4.1

Comparison biases and uncertainties

Table B.6. estimated uncertainties on isotopic concentrations for GU3', taking into account the calculation bias and the experimental and calculated uncertainties. ΔC_{max} come from the nuclear data library leading to the highest nuclear data uncertainty (either ENDF/B-VIII.0, JEFF-3.3 or JENDL-4.0).

	Bias (%)	ΔE (%)	ΔC_{max} (%)
^{234}U	+44	2.5	7.9
^{236}U	+0.7	0.4	1.7
^{237}Np	−14	3.8	4.2
^{239}Pu	−0.3	0.3	3.2
^{241}Pu	−3.1	0.3	4.2
^{244}Pu	−73	25	9.7
^{242m}Am	+8.5	5.5	6.6
^{242}Cm	−6.1	3.6	1.6
^{244}Cm	−11	1.8	11
^{246}Cm	−20	5.2	25
^{90}Sr	+5.4	8.0	1.4
^{99}Tc	−8.5	8.9	1.7
^{106}Ru	−3.6	14	1.9
^{109}Ag	−35	9.1	20.9
^{129}I	−17	5.6	6.1
^{134}Cs	−1.6	1.5	30
^{137}Cs	+1.7	2.4	6.9
^{142}Nd	+0.5	5.0	5.3
^{144}Nd	−0.4	0.3	2.4
^{146}Nd	−0.5	0.3	1.9
^{150}Nd	−0.1	0.3	1.2
^{147}Sm	+9.2	0.3	2.4
^{149}Sm	+9.6	1.0	4.5
^{151}Sm	+0.1	0.4	12
^{154}Sm	+10	0.3	7.4
^{154}Eu	+6.0	1.9	3.7
^{155}Gd	−14	1.1	24

	Bias (%)	ΔE (%)	ΔC_{max} (%)
^{235}U	+3.0	0.4	3.1
^{238}U	+0.0	0.2	0.0
^{238}Pu	−5.8	1.5	10
^{240}Pu	+2.2	0.3	4.5
^{242}Pu	+0.0	0.3	8.7
^{241}Am	+14	1.8	5.1
^{243}Am	−1.0	1.8	9.3
^{243}Cm	+38	10	16
^{245}Cm	−8.6	2.6	17
^{95}Mo	−11	4.6	1.1
^{101}Ru	−12	12	3.1
^{103}Rh	+23	4.9	1.8
^{125}Sb	+63	9.4	30
^{133}Cs	+7.2	1.5	30
^{135}Cs	+5.4	1.5	20
^{144}Ce	+3.9	1.7	1.0
^{143}Nd	+3.1	0.3	3.7
^{145}Nd	+1.1	0.3	2.0
^{148}Nd	+0.5	0.3	0.9
^{147}Pm	+23	9.0	2.6
^{148}Sm	−4.0	0.3	2.4
^{150}Sm	+5.6	0.3	1.5
^{152}Sm	+6.2	0.3	4.0
^{153}Eu	−1.7	0.3	3.4
^{155}Eu	−8.3	5.0	24

Conclusions

- GU3 is relatively challenging due to its relocation
- GU3' seems more trusted than GU3

- Nuclear data libraries affect the C/Es
- Nuclear data uncertainties are different based on different libraries
- The effect of fission yields is not negligible (which sampling method for the SG10 follow-up?)

- Other sources of uncertainties can be as large as the ones from nuclear data
- Not all biases can be explained by calculated uncertainties: necessity to consider many samples in validation studies.

- Same methods applied to
  - GU3: https://www.epj-n.org/articles/epjn/pdf/2021/01/epjn210012.pdf.
  - GU1: https://www.sciencedirect.com/science/article/pii/S0306454921002358.
  - U1: https://www.sciencedirect.com/science/article/pii/S0306454920304047.
  - BM1 & BM3: https://www.epj-n.org/articles/epjn/abs/2021/01/epjn210030/epjn210030.html.
  - ENRESA: https://www.epj-n.org/articles/epjn/abs/2022/01/epjn220015/epjn220015.html.

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Wir schaffen Wissen – heute für morgen