SCALE-6.3.0/Polaris-PARCS-v3.4.2 Validation: Reactor Physics

April 27, 2023

2023 SCALE Users' Group Workshop

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Contents

- **SCALE-6.3.0/Polaris Validation**
  - Benchmark for the critical experiments: CE, B&W-1810 and KRITZ
  - Pin power uncertainty analysis
- **LWR Power Plant Benchmarks**
  - PWR validation: Watt Bar 1, BEAVRS
  - BWR validation: Peach Bottom Unit 2, Hatch 1
- **Discussion**
  - Pending issues in Polaris and PARCS
  - Additional LWR plants
- **Conclusion**
  - Final goal
- **Future Work**

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Polaris Validation

- **Objectives**
  - Validate the SCALE-6.3.0/Polaris with the ENDF/B-VII.1 AMPX 56-group library through the benchmark calculations for critical experiments
  - Assess the pin-to-box factor uncertainty
  - Eigenvalues with the measured bucklings
- **Code and library**
  - SCALE-6.3.0/Polaris
  - ENDF/B-VII.1 AMPX 56-group library
  - VERA MPACT with the ENDF/B-VII.1 MPACT 51-group library
- **Critical experiments**
  - CE critical experiments (5): #12, 43, 32, 53, 56
  - B&W-1810 critical experiments (6): #1, 5, 12, 14, 18, 20
  - KRITZ critical experiments (5): #1, 2, 3, 4, 5

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CE Critical Experiments

Type	Temperature (°C)	Boron Concentration (ppm)	Axial Buckling (cm^{-2})
Core 12	20.0	0	0.003450
Core 32		0	0.003580
Core 43		323	0.001620
Core 53		0	0.002850
Core 56		302	0.001080

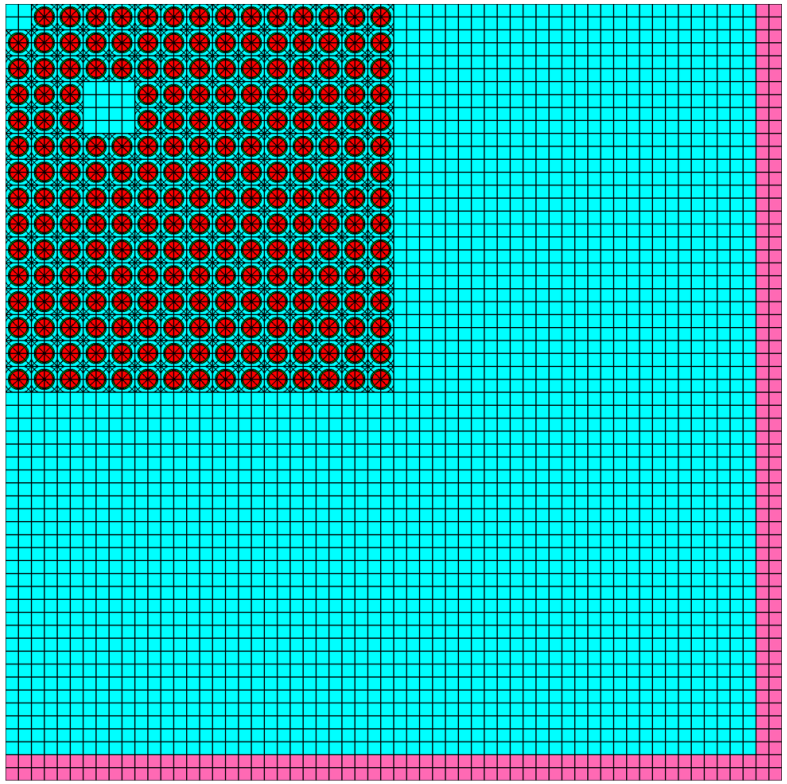

Figure 2.1 Configuration of the CE critical cores #12 and #43

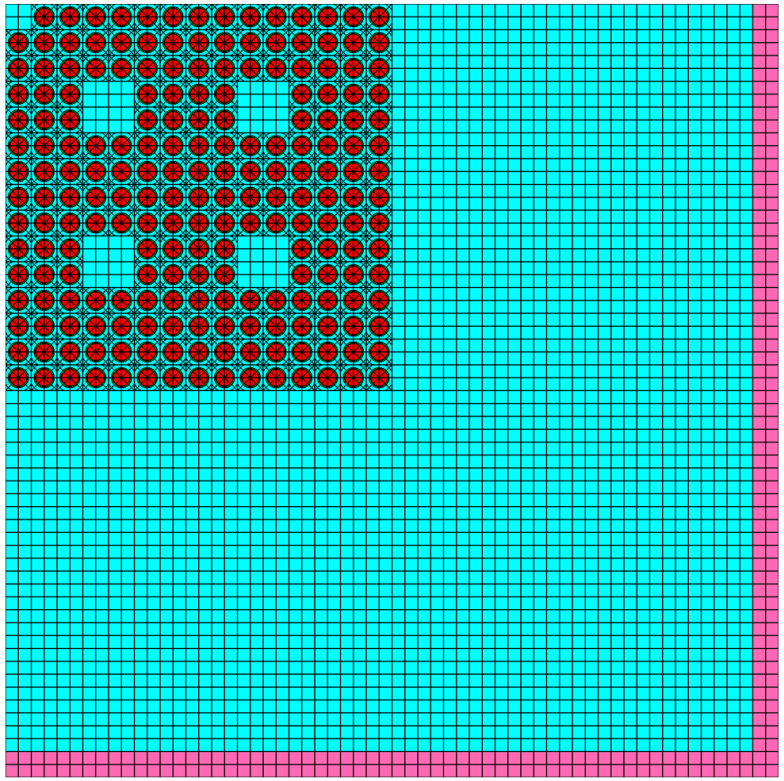

Figure 2.2 Configuration of the CE critical cores #32, #53 and #56

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B&W-1810 Critical Experiments

Type	Temperature(°C)	Boron Concentration (ppm)	Axial Buckling (cm^{-2})
Core 1	25.0	1337.9±0.4	0.000350 (0.00041 CASMO)
Core 5		1208.0±0.4	
Core 12		1899.3±0.9	
Core 14		1653.8±0.7	
Core 18		1776.8±1.0	
Core 20		1499.0±0.6	

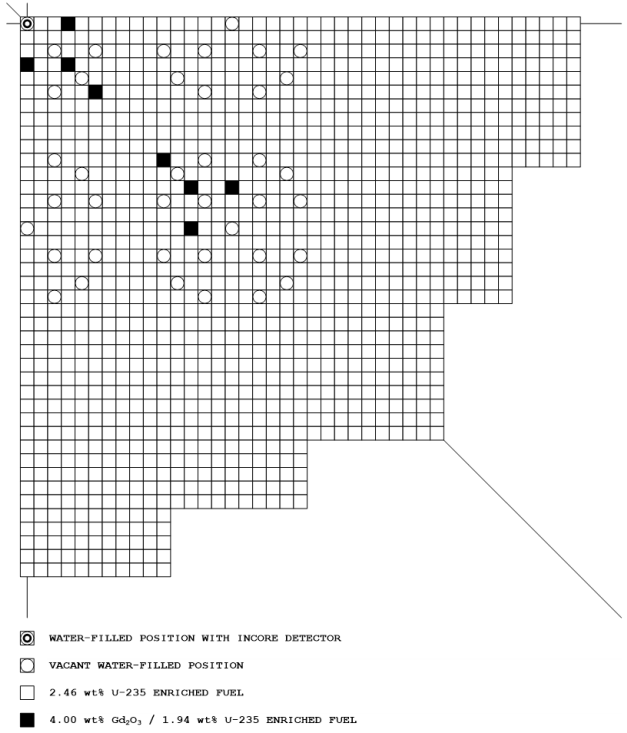
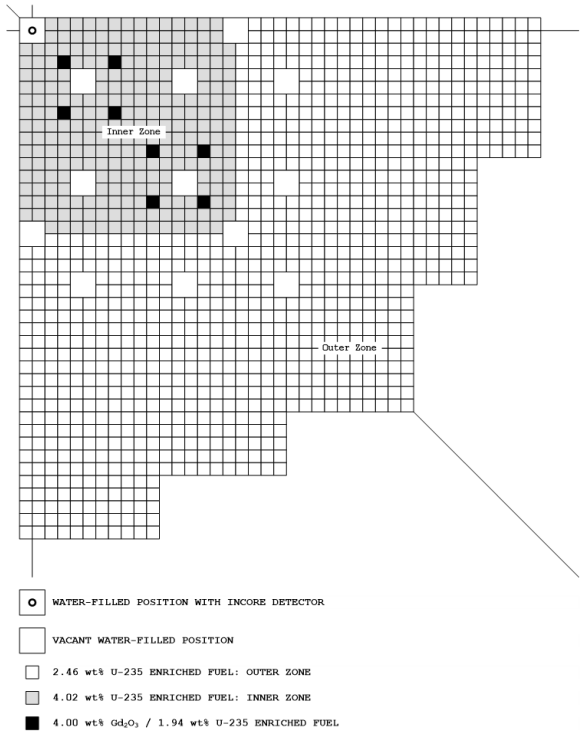


Figure 2.4 Configuration of the B&W critical core #5



igure 2.8 Configuration of the B&W critical core #20

Core	Description	Number of rods							Boron (ppm)
		2.46%	4.02%	Gd	B_4C	AIC	Void	Water	
1	0 Gd	4808	-	-	-	-	-	153	1337.9
2	0Gd, AIC	4808	-	-	-	16	-	137	1250.0
3	20 Gd	4788	-	20	-	-	-	153	1239.3
4	20 Gd, AIC	4788	-	20	-	16	-	137	1171.7
5	28 Gd	4780	-	28	-	-	-	153	1208.0
5A	32 Gd	4776	-	32	-	-	-	153	1191.3
5B	28 Gd	4780	-	28	-	-	-	153	1207.1
6	28 Gd, AIC	4780	-	28	-	16	-	137	1155.8
6A	32 Gd, AIC	4776	-	32	-	16	-	137	1135.6
7	28 Gd (annular)	4780	-	28	-	-	-	153	1208.8
8	36 Gd	4772	-	36	-	-	-	153	1170.7
9	36 Gd, AIC	4772	-	36	-	16	-	137	1130.5
10	36 Gd, Void	4772	-	36	-	-	16	137	1177.1
12	0 Gd	3920	888	-	-	-	-	153	1899.3
13	0 Gd, B_4C	3920	888	-	16	-	-	137	1635.4
14	28 Gd	3920	860	28	-	-	-	153	1653.8
15	28 Gd, B_4C	3920	860	28	16	-	-	137	1479.7
16	36 Gd	3920	852	36	-	-	-	153	1579.4
17	36 Gd, B_4C	3920	852	36	16	-	-	137	1432.1
18	16x16	3676	944	-	-	-	-	180	1776.8
19	16x16	3676	928	16	-	-	-	180	1628.3
20	16x16	3676	912	32	-	-	-	180	1499.8

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KRITZ Critical Experiments

Type	Temperature (°C)	Boron Concentration (ppm)	Axial Buckling (cm^{-2})
Core 1 (U-WH1)	229.0	1006	0.000182
Core 2 (Pu-WH1)	223.2	990	0.000307
Core 3 (U-WH2)	228.7	959	0.000220
Core 4 (Pu-WH2, Cold)	24.6	1122	0.000178
Core 5 (Pu-WH2, Hot)	230.7	949	0.000270

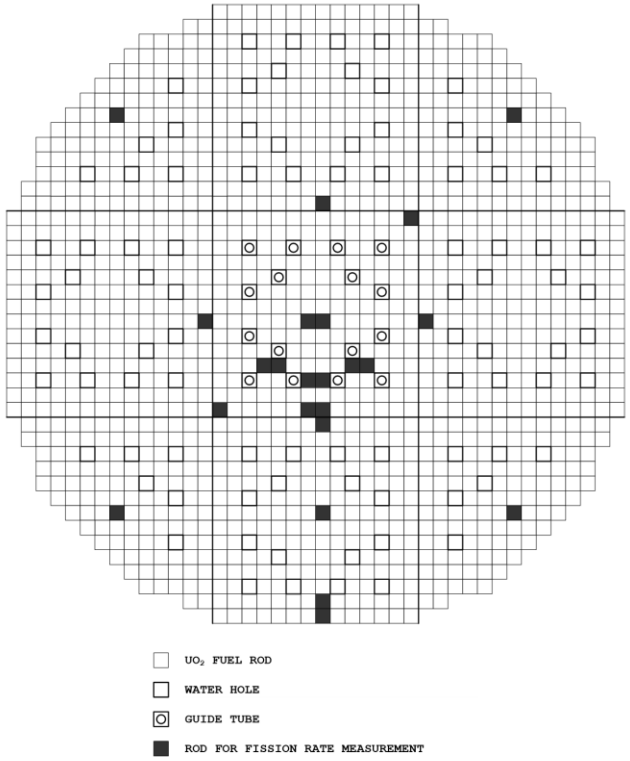

Figure 2.10 Configuration of the KRITZ critical core #1

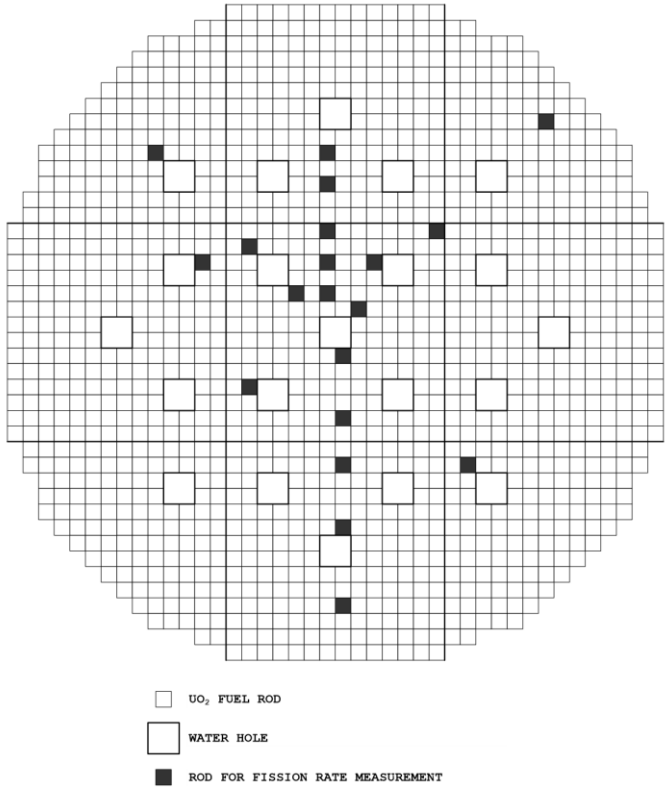

Figure 2.12 Configuration of the KRITZ critical core #3

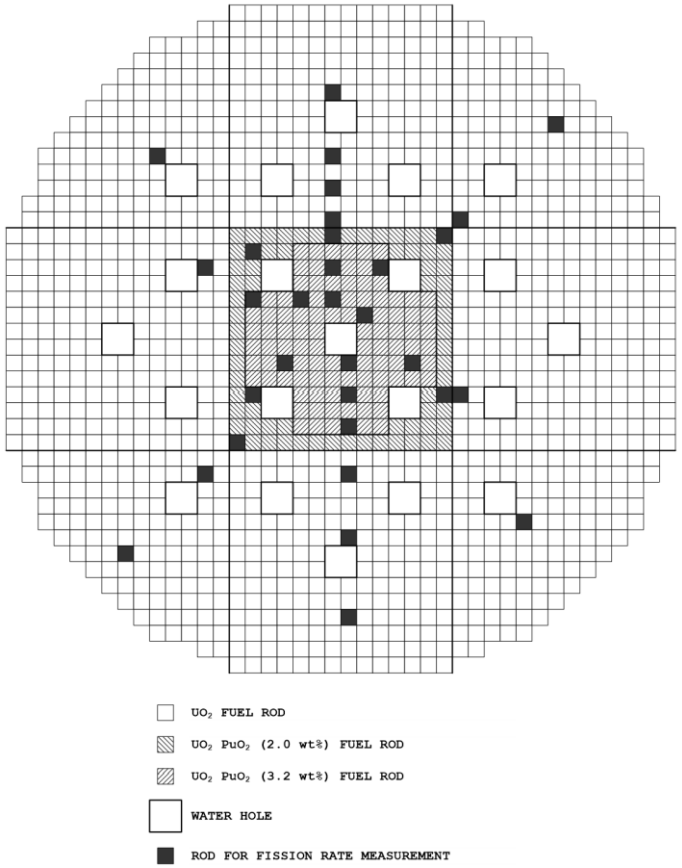

Figure 2.14 Configuration of the KRITZ critical core #5

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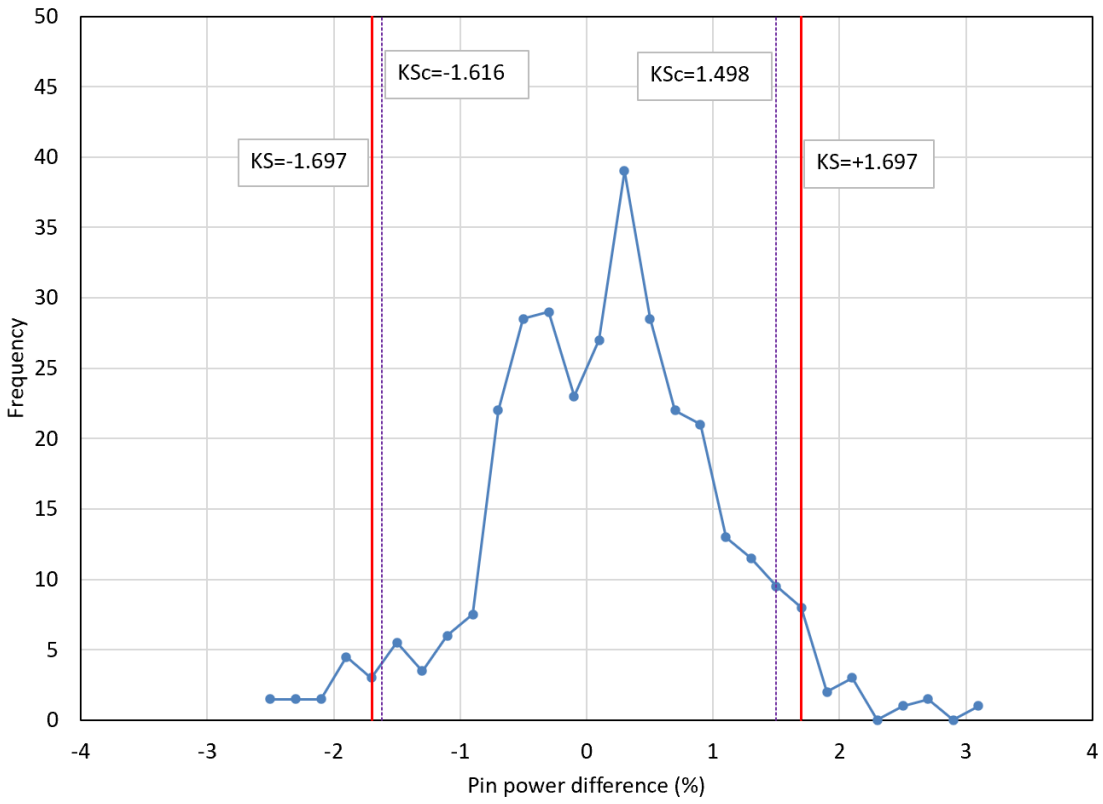
Polaris Pin Power Uncertainty

Experiments	S_d	F_d	S_m	F_m	S_c	F_c
CE12	0.947	21	1.040	19	-	-
CE32	1.076	21	0.661	19	0.849	10
CE43	0.900	21	0.867	19	0.240	2
CE53	0.616	21	0.988	19	-	-
CE56	0.679	21	0.594	19	0.329	3
All	0.861	105	0.848	95	0.699	15
BAW01	0.504	25	0.168	64	0.449	16
BAW05	0.637	25	0.381	64	0.357	3
BAW12	0.730	25	0.435	64	0.538	8
BAW14	1.026	25	0.491	64	0.617	3
BAW18	1.181	28.5	0.772	64	0.382	0
BAW20	1.479	28.5	0.584	64	0.809	3
All	1.004	157	0.507	384	0.520	32
KRITZ01	0.411	3.5	0.000	0	0.590	3.5
KRITZ02	1.060	9.5	0.000	0	0.515	9.5
KRITZ03	0.896	8	0.000	0	1.191	8
KRITZ04	1.081	14	0.000	0	1.144	14
KRITZ05	0.698	13	0.000	0	1.309	13
All	0.917	48	0.000	0	1.077	48
S_p(All)	0.944	310	0.590	479	0.867	96
K_{95x95}	1.797		1.766		1.896	
K_{95x95}*Sp	1.697		1.043		1.644	

$$S_c^2(pin) = S_c^2(box) + S_c^2(pin-to-box)$$



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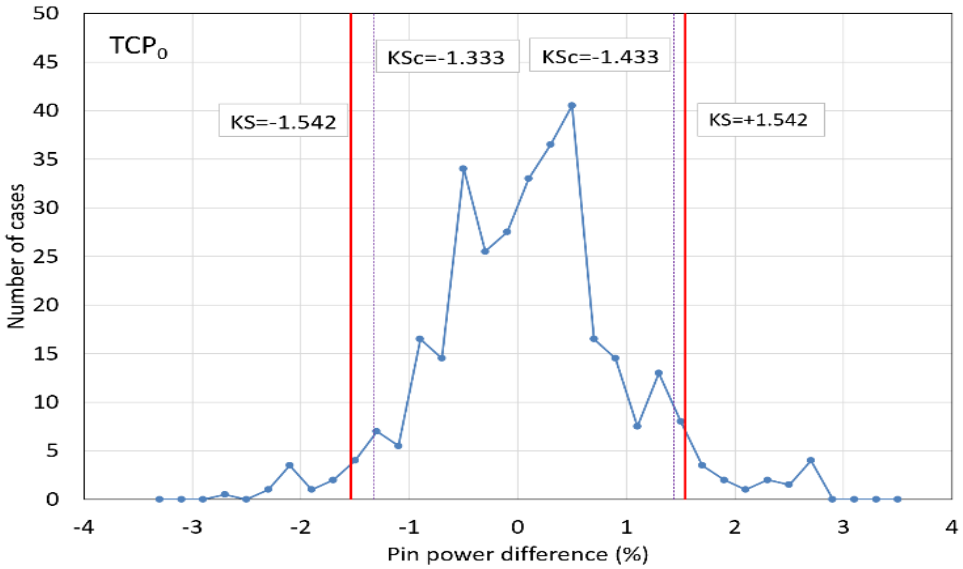
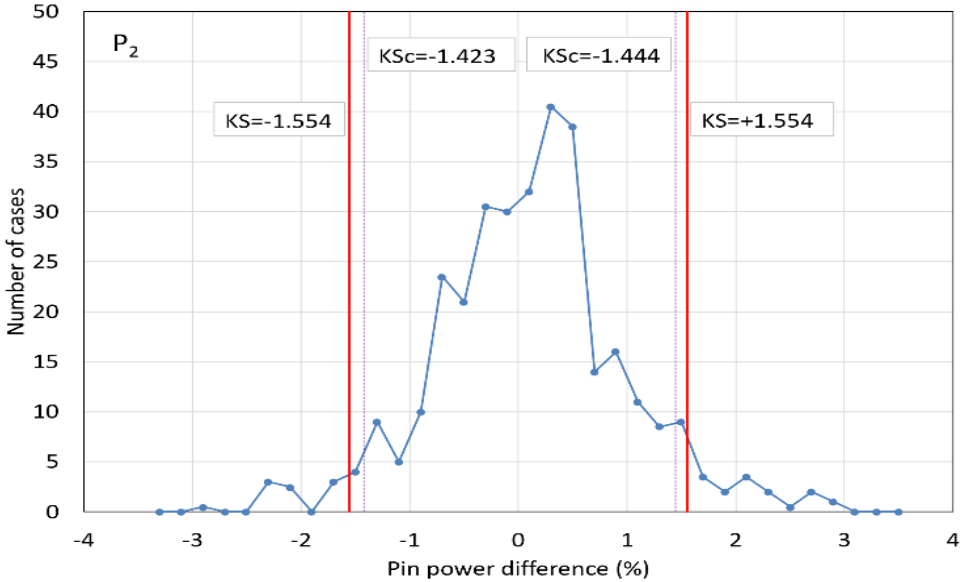
VERA-MPACT Pin Power Uncertainty

Case	Core	TCP_0		P_2		Measured	
		S_d	F_d	S_d	F_d	S_m	F_m
CE	12	0.968	21	0.960	21	1.040	19
	32	1.093	21	1.072	21	0.661	19
	43	0.858	21	0.889	21	0.867	19
	53	0.689	21	0.682	21	0.988	19
	56	0.780	21	0.766	21	0.594	19
	All	0.889	105	0.885	105	0.848	95
B&W	1	0.480	25	0.492	25	0.168	64
	5	0.522	25	0.526	25	0.381	64
	12	0.692	25	0.721	25	0.435	64
	14	0.789	25	0.812	25	0.491	64
	18	0.862	28.5	0.867	28.5	0.772	64
	20	0.998	28.5	0.959	28.5	0.584	64
	All	0.756	157	0.757	157	0.507	384
KRITZ	1	0.590	3.5	0.593	3.5	–	–
	2	0.515	9.5	0.564	9.5	–	–
	3	1.191	8	1.188	8	–	–
	4	1.144	14	1.157	14	–	–
	5	1.309	13	1.397	13	–	–
	All	1.077	48	1.115	48	–	–
S_p (All)		0.858	310	0.865	310	0.590	479
$K_{95\times95}$		1.797		1.797		1.766	
$K_{95\times95}S_p$		1.542		1.554		1.043	





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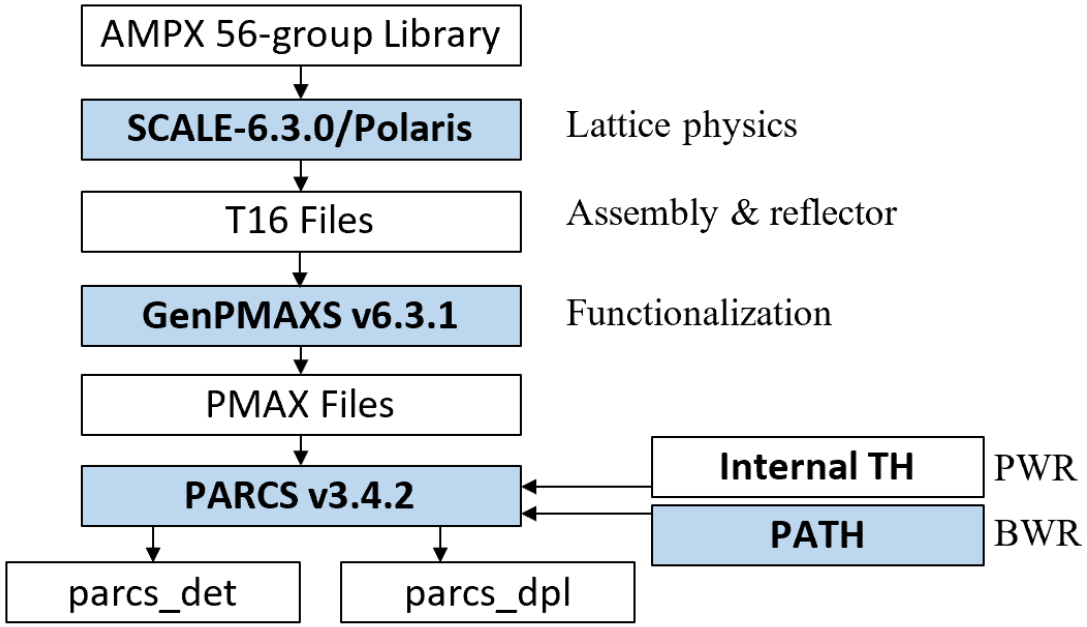
SCALE-6.3.0/Polaris-PARCS v3.4.2 Validation

- **Codes and Libraries**
  - SCALE-6.3.0/Polaris with the ENDF/B-VII.1 AMPX 56-group library
  - GenPMAXS v6.3.1
  - PARCS v3.4.2

- **LWR benchmarks**
  - 2 PWRs with 5 cycles: Watt Bar 1 (3), BEAVRS (2)
  - 2 BWRs with 6 cycles: Peach Bottom 2 (3), Hatch (3)
  - At least 20 cycles for each LWR type



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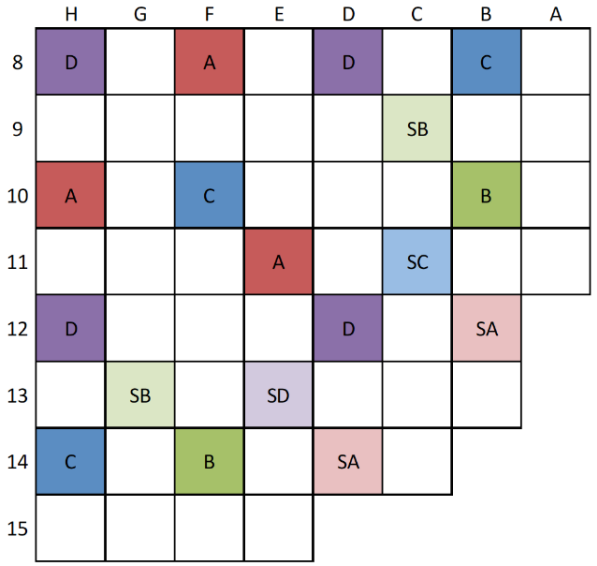
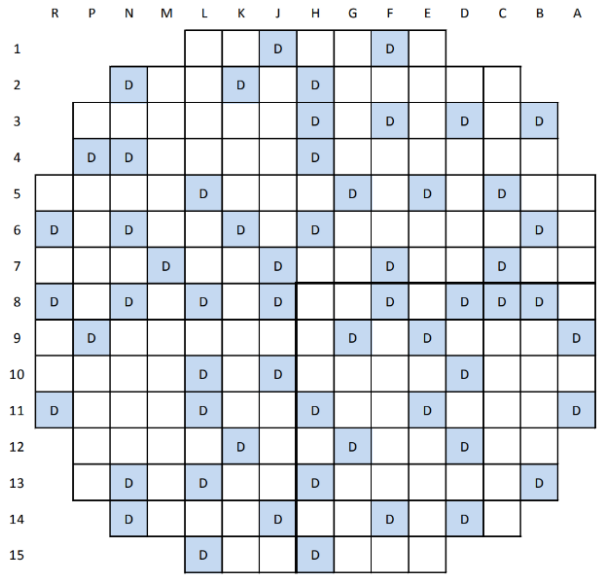
PWR :: Watt Bar 1 Cycles 1-3

Table 3.2 Specification of the WBN1 core

Parameter	Design data	Remarks
Core power	3411 MWth	
Operating pressure	2250 psia (15.51 MPa)	
Core flow rate	59.738×10^6 kg/hr (144.7 Mlbs/hr)	9% bypass
Inlet temperature	565 K (291.85 °C)	
Number of fuel assemblies	193	
Region 1 (cycle 1)	2.11 w/o ^{235}U	
Region 2 (cycle 1)	2.619 w/o ^{235}U	
Region 3 (cycle 1)	3.10 w/o ^{235}U	
Region 4 (cycle 2)	3.709 w/o ^{235}U	
Total heavy metal mass (cycle 1)	- MT	
Pin lattice configuration	17×17	
Active fuel length	365.76 cm	
Number of fuel rods	264	
Number of grid spacers	8	6 Zircaloy, 2 Inconel-718
Assembly pitch	21.50 cm	
Pin pitch	1.260 cm	
Fuel pellet radius	0.4096 cm	
Cladding inner/outer radius	0.4180/0.4750 cm	
Number of control banks	57	
Control rod material (upper)	B_4C	
Control rod material (lower)	AgInCd	
Number of burnable poison rods	1266	
Burnable poison material	Borosilicate glass, 12.5 w/o B_2O_3	Cycle 1
	IFBA & WABA	Cycle 2





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PWR :: Watt Bar 1 Cycles 1-3

	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1	3.1 16	3.1	3.1		
15	3.1 12	3.1	3.1 8	3.1				

Enrichment
Number of Pyrex Rods

	H	G	F	E	D	C	B	A
8	H-14	N-13	128*	R-8	128	N-8	L-15	F-11
9	N-3	104	A-9	104|8	B-11	128*	48	C-4
10	128*	G-15	E-15	D-7	104|8	B-7	48	G-10
11	H-1	104|8	J-12	128*	N-2	128	48	F-13
12	128	E-14	104|8	P-3	A-6	104|4	B-4	
13	H-3	128*	J-14	128	104|4		P-6	
14	R-5	48	48	48	M-14	K-2		
15	L-10	M-13	F-9	C-10				

IFBA|WABA or
Previous Cycle 1 Location

* 132 inch IFBA (All others 120 inch)

Batch 1 - 2.11%
Batch 2 - 2.619%
Batch 3 - 3.1%
Batch 4 - 3.709%

	H	G	F	E	D	C	B	A
8	1A-10	H-6	5A 128	L-5	N-13	D-8	5A 104	J-9
9	F-8	5B 128	D-13	5B 128	B-7	5A 104	5B 128	M-10
10	5A 128	C-12	L-2	N-11	5B 128	G-11	5B 128	M-2
11	E-5	5B 128	E-3	5B 128	J-3	5A 128	5B 16	A-5
12	N-3	J-14	5B 128	N-7	E-2	5B 128	P-10	
13	H-12	5A 104	E-9	5A 128	5B 128	5B 16	G-15	
14	5A 104	5B 128	5B 128	5B 16	F-2	A-9		5A
15	J-7	F-4	P-4	L-15				5B

Batch 5A – 3.8%
Batch 5B – 4.4%

1A-10: from cycle-1

- **Measured data**
  - Cycles 1-3: available for public through OECD/NEA UAM
    - HZP physics test results, critical boron concentration, flux maps
  - Cycles 4-12: available for CASL

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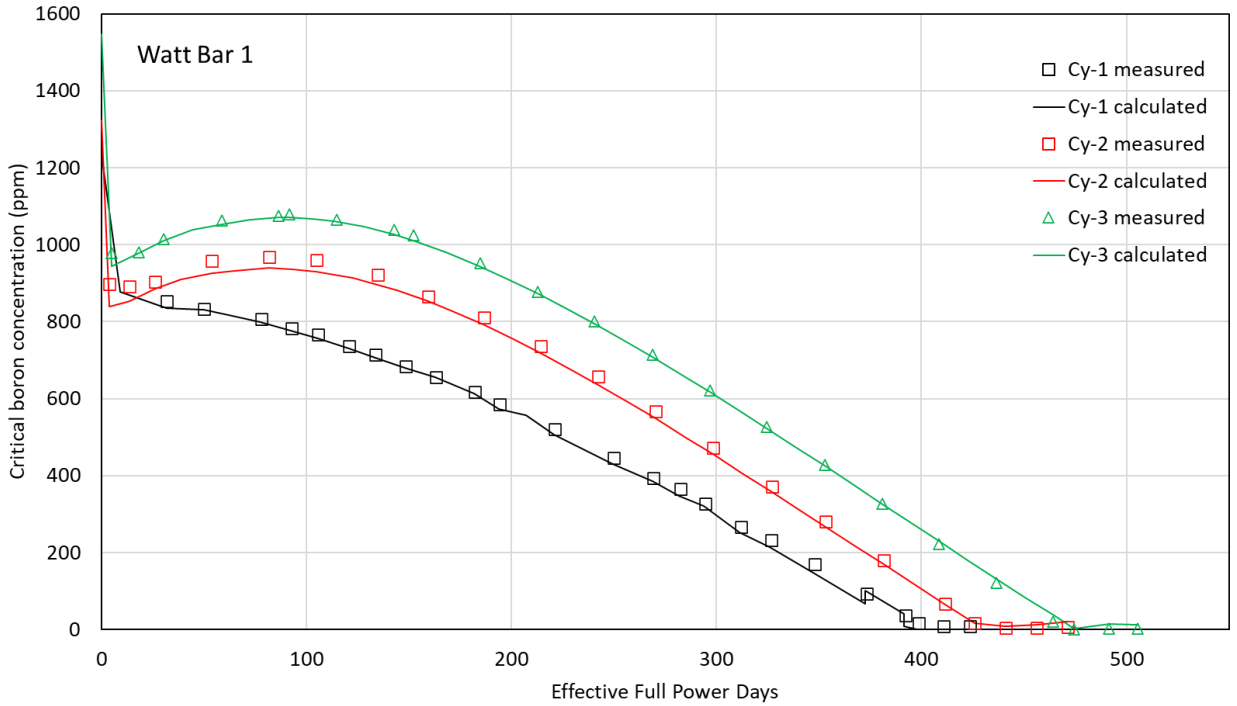
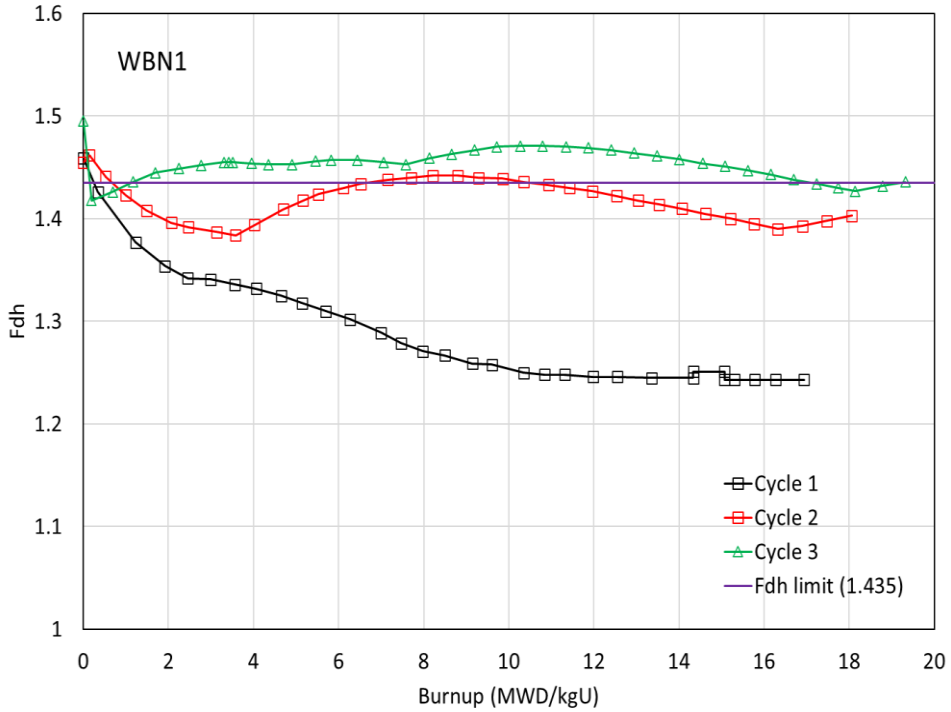
PWR :: Watt Bar 1 Cycles 1-3

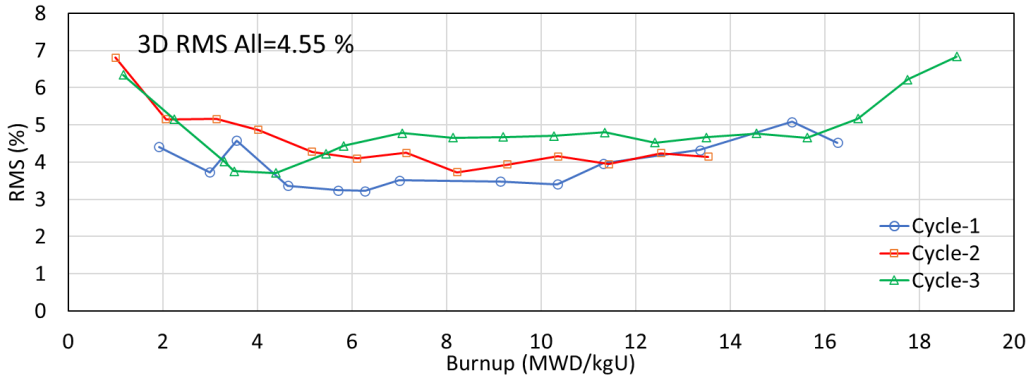
Table 3.4 Comparison of the control bank worth and ITC for WBN1

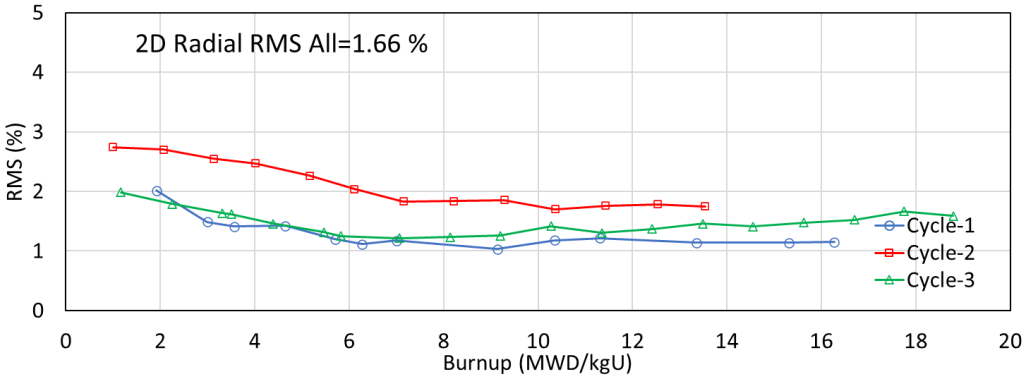
Cycle	Case	Critical boron (ppm)		Control bank worth (pcm)			ITC (pcm/°F)			Boron worth (pcm/ppm)		
		Meas.	Calc.	Meas.	Calc.	Diff.	Meas.	Calc.	Diff.	Meas.	Calc.	Diff.
1	ARO	1291					-2.2	-3.39	-1.19	-10.77	-10.18	0.59
	A			843	977	134						
	B			879	840	-39						
	C			951	1031	80						
	D			1342	1450	108						
	SA			435	421	-14						
	SB			1056	1077	21						
	SC			480	458	-22						
	SD			480	458	-22						
	All			6466	6713	247						

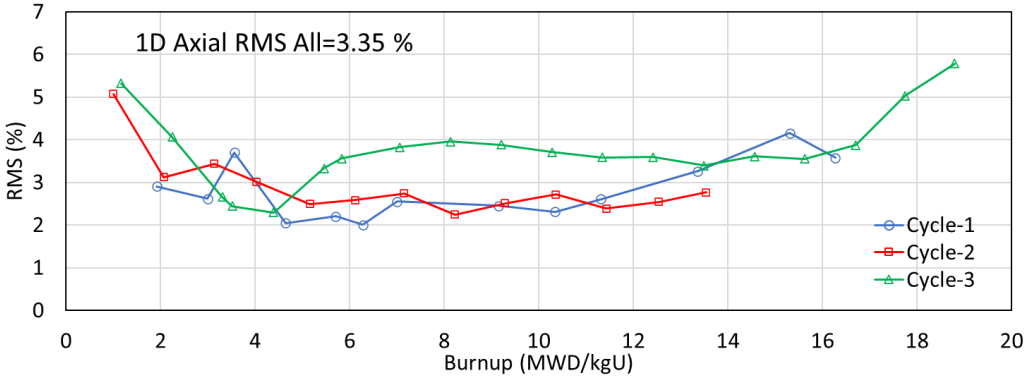




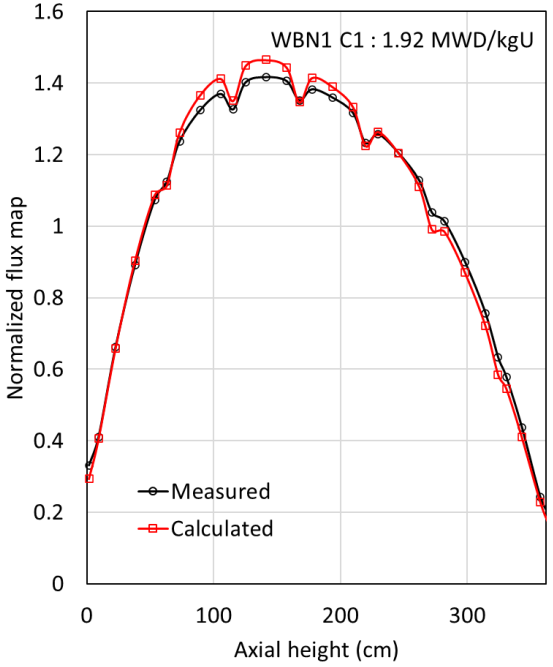
PWR :: Watt Bar 1 Cycles 1-3

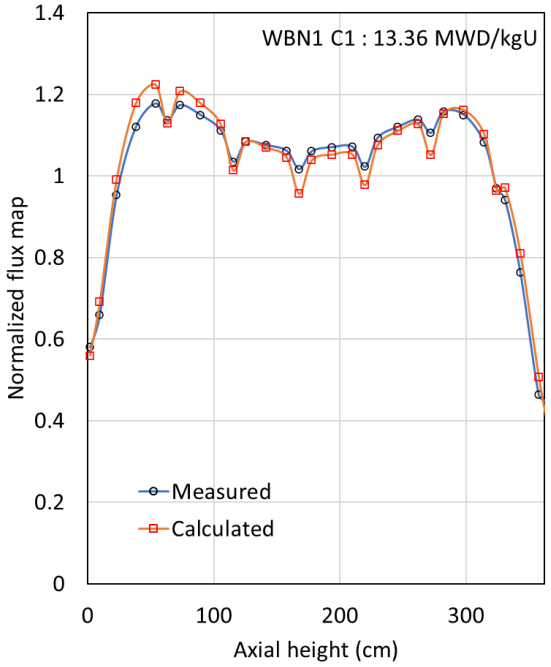






Cycle	VERA RMS %			Polaris-PARCS RMS %		
	3D	2D	1D	3D	2D	1D
1	3.0	1.3	1.8	4.0	1.3	2.9
2	3.2	1.9	1.4	4.6	2.1	3.0
3	3.3	1.5	2.4	4.9	1.5	3.9





- **Needs to improve axial power shape**
  - Axial reflector models
  - Inc-718 space grid model

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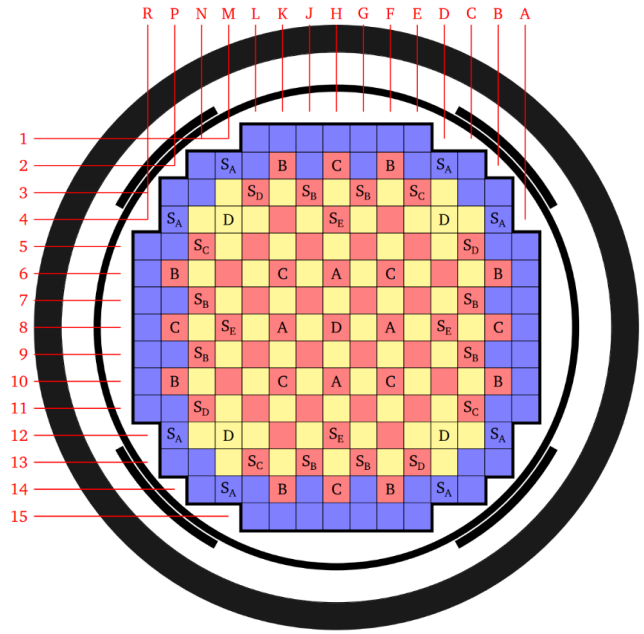
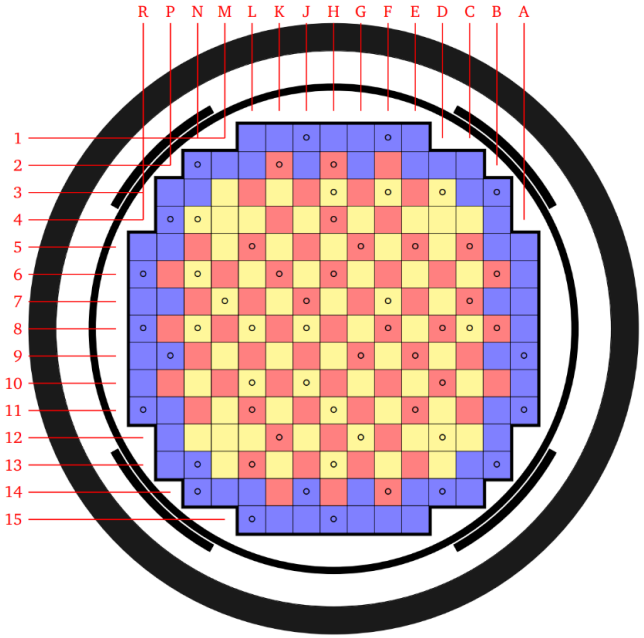
PWR :: BEAVRS Cycles 1-2

Table 3.6 Specification of the BEAVRS core

Parameter	Design data	Hot dimension
Core power	3411 MWth	
Operating pressure	2250 psia (15.51 MPa)	
Core flow rate	61.5×10^{6} kg/hr (5% bypass)	
Inlet temperature	292.89 °C	
Number of fuel assemblies	193	
Region 1 (cycle 1)	1.60 w/o ^{235}U	
Region 2 (cycle 1)	2.40 w/o ^{235}U	
Region 3 (cycle 1)	3.10 w/o ^{235}U	
Region 4A (cycle 2)	3.20 w/o ^{235}U	
Region 4B (cycle 2)	3.40 w/o ^{235}U	
Total heavy metal mass (cycle 1)	81.8 MT	
Pin lattice configuration	17×17	
Active fuel length	365.76 cm	367.6833 cm
Number of fuel rods	264	
Number of grid spacers	8 (6 Zircaloy, 2 Inconel-718)	
Assembly pitch	21.50364 cm	21.60912 cm
Pin pitch	1.25984 cm	1.26198 cm
Fuel pellet radius	0.39218 cm	0.39424 cm
Cladding inner/outer radius	0.40005/0.45720 cm	0.40073/0.45798 cm
Number of control banks	57	
Control rod material (upper)	B_4C	
Control rod material (lower)	AgInCd	
Number of burnable poison rods	1266	
Burnable poison material	Borosilicate glass, 12.5 w/o B_2O_3	





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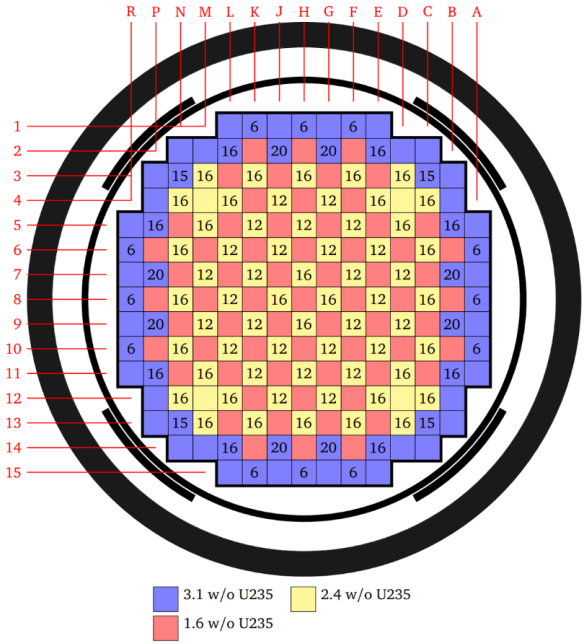
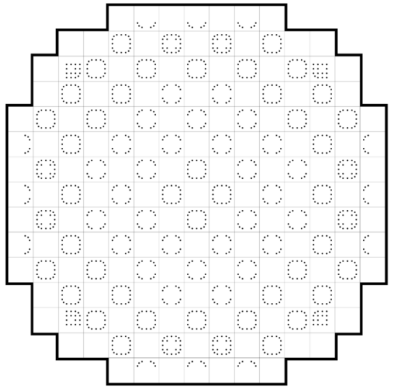
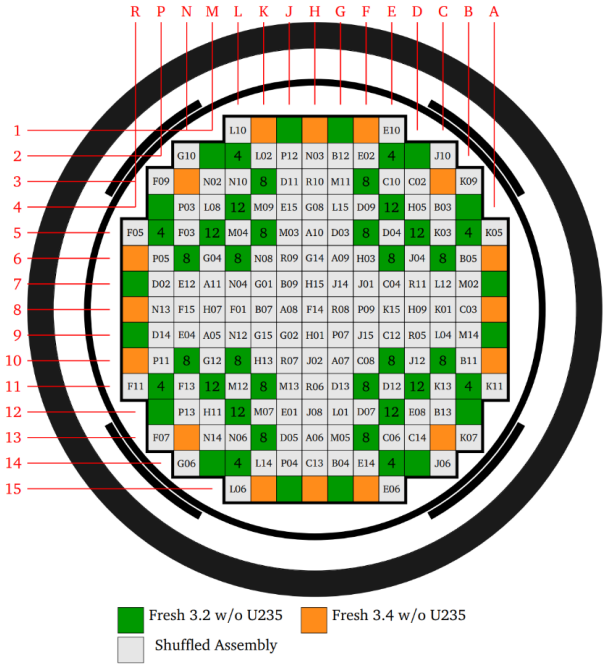
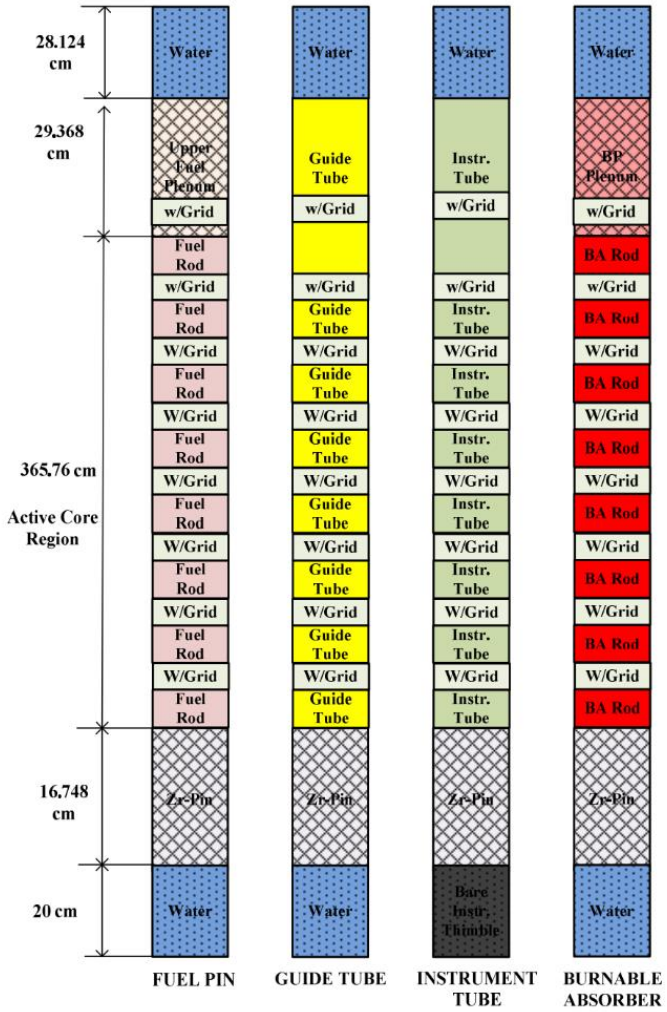
PWR :: BEAVRS Cycles 1-2









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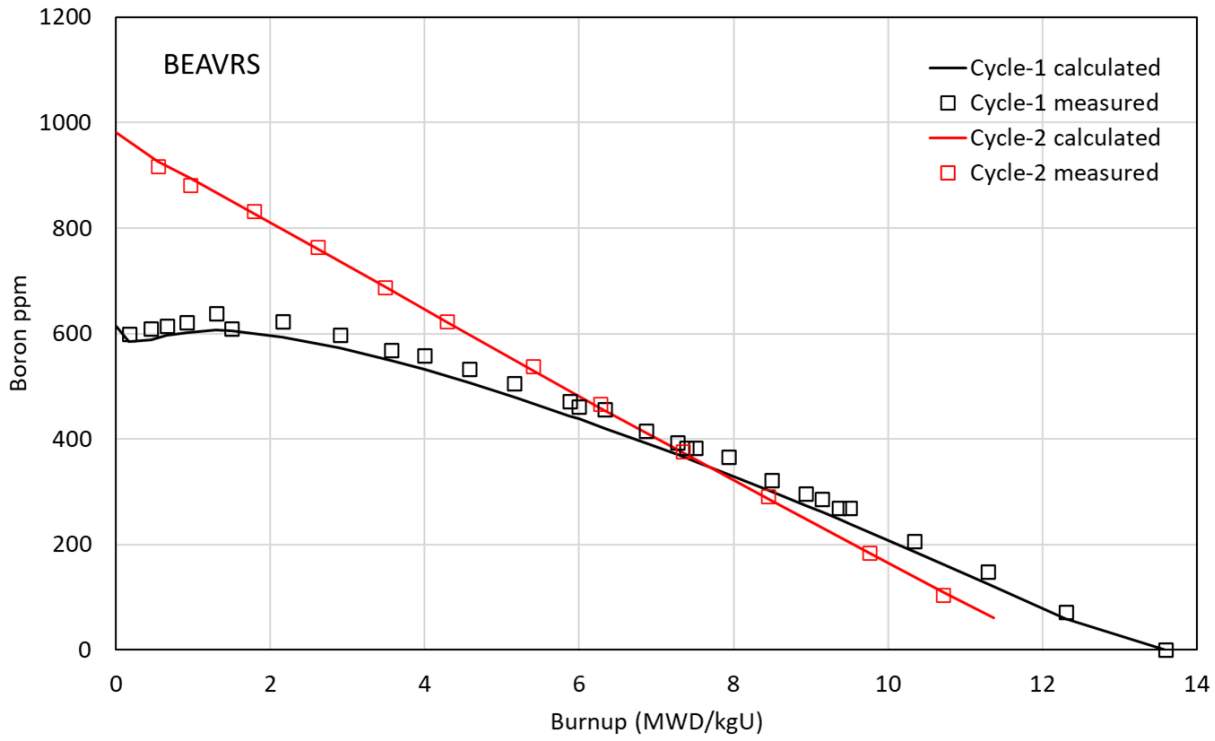
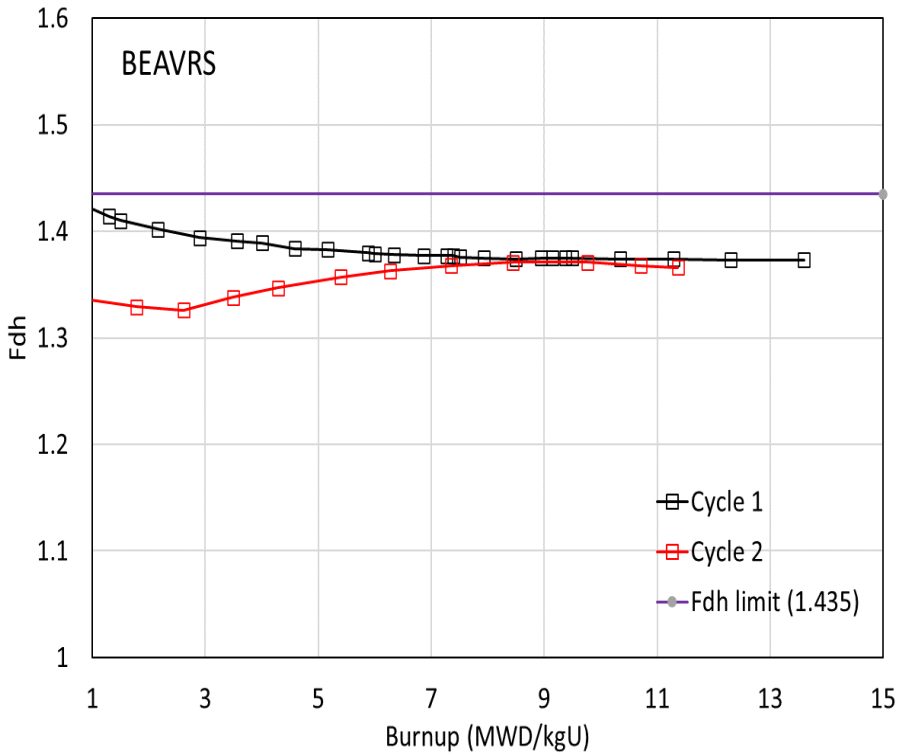
PWR :: BEAVRS Cycles 1-2

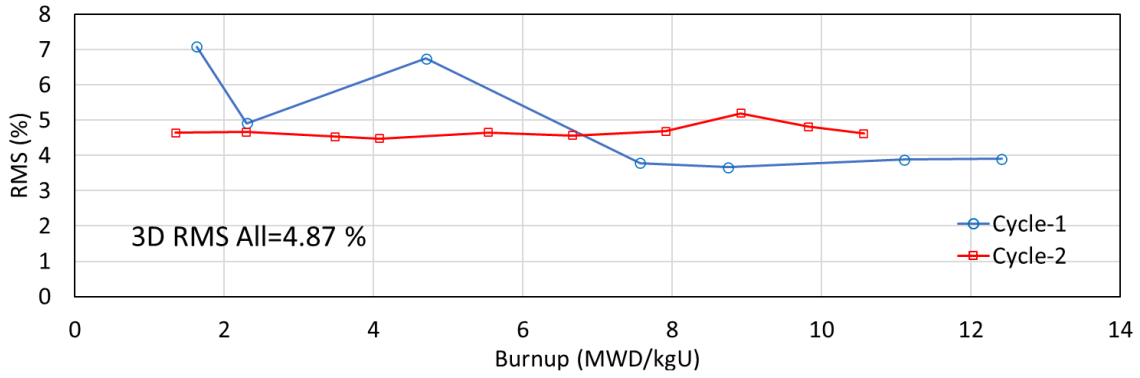
Table 3.7 Comparison of the control bank worth and ITC for the BEAVRS cycle 1

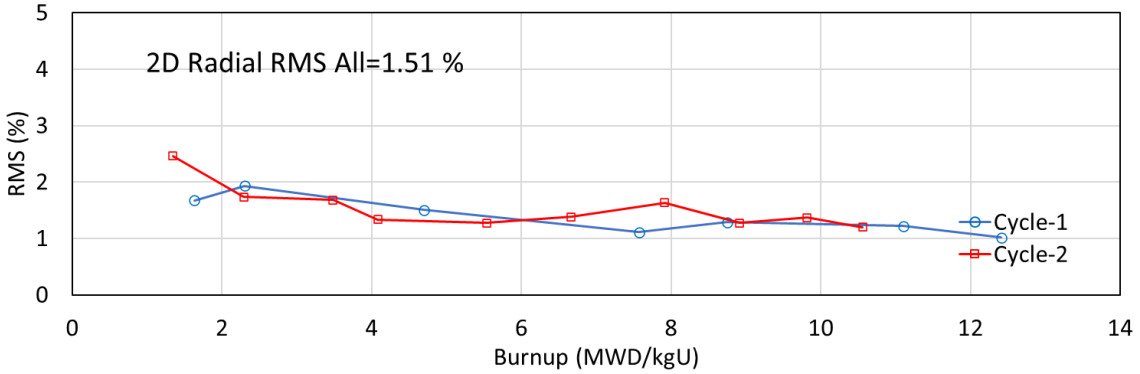
Case	Critical boron (ppm)		Control bank worth (pcm)			ITC (pcm/°F)		
	Meas.	Calc.	Meas.	Calc.	Diff.	Meas.	Calc.	Diff.
ARO	975	957.8				-1.75	-2.03	-0.28
D with ARO	902	896	788	793.5	5.5	-4.65	-3.49	1.16
C with D in	810	794.7	1203	1275.7	72.7	-8.01	-8.27	-0.26
B with D+C in		703	1171	1213.3	42.3			
A with D+C+B in	686	655	548	614.5	66.5			
SE with D+C+B+A in		612.5	461	525.6	64.6			
SD with D+C+B+A+SE in		551.7	772	755.6	-16.4			
SC with D+C+B+A+SE+SD in	508	463.7	1099	1111.7	12.7			

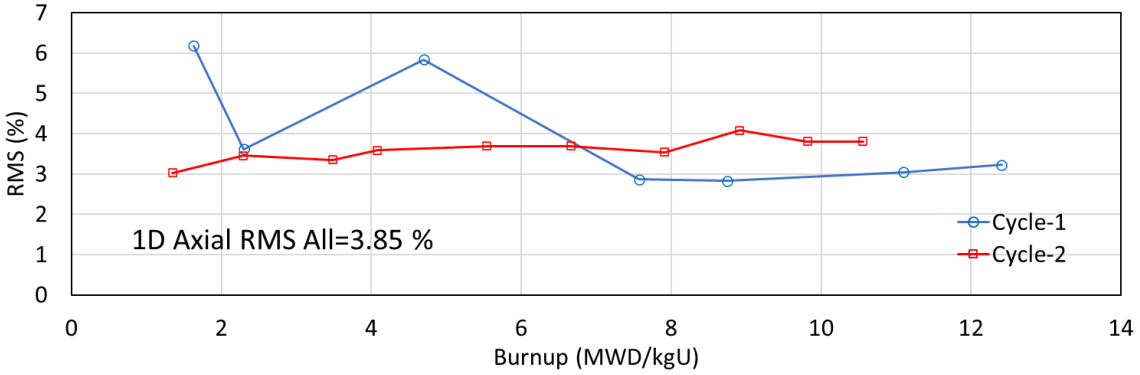




PWR :: BEAVRS Cycles 1-2

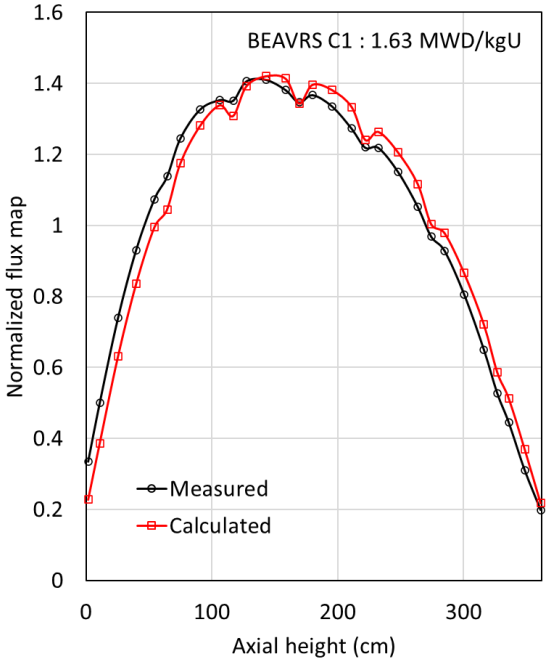


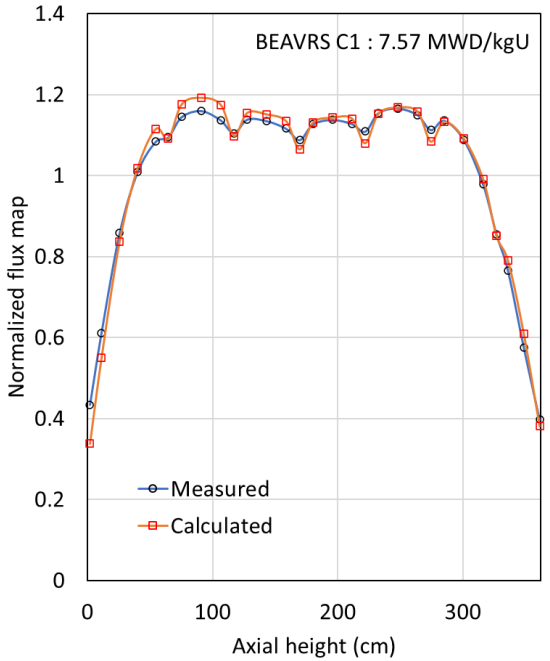




-	0.779	1.065	0.940	1.147	0.935	1.264	0.778
0.949	0.789	1.072	0.937	1.154	0.943	1.268	0.770
-	1.00	0.65	-0.32	0.71	0.78	0.37	-0.81
Meas.	1.011	0.897	1.143	0.974	1.168	0.873	0.815
Calc.	1.025	0.907	1.150	0.968	1.195	0.876	0.790
% diff	1.35	0.96	0.67	-0.63	2.73	0.28	-2.51
	0.897	1.138	0.968	1.212	0.984	1.242	0.728
	0.907	1.146	0.983	1.205	0.977	1.260	0.717
	0.96	0.85	1.52	-0.74	-0.69	1.77	-1.14
	1.143	0.968	1.249	-	1.307	-	0.584
	1.150	0.983	1.257	1.072	1.344	0.923	0.568
	0.68	1.52	0.85	-	3.73	-	-1.64
	0.974	1.212	-	1.343	1.196	0.958	
	0.968	1.205	1.072	1.337	1.199	0.910	
	-0.63	-0.74	-	-0.64	0.31	-4.78	
	1.168	0.984	1.307	1.196	0.852	0.702	
	1.195	0.977	1.344	1.199	0.934	0.649	
	2.73	-0.69	3.73	0.32	8.17	-5.27	
	0.873	1.242	-	0.958	0.702		
	0.876	1.260	0.923	0.910	0.649		
	0.28	1.77	-	-4.78	-5.27		
	0.815	0.728	0.584				
	0.790	0.717	0.568				
	-2.51	-1.14	-1.63				

Figure 3.12 BEAVRS cycle-1 HZP detector response comparison





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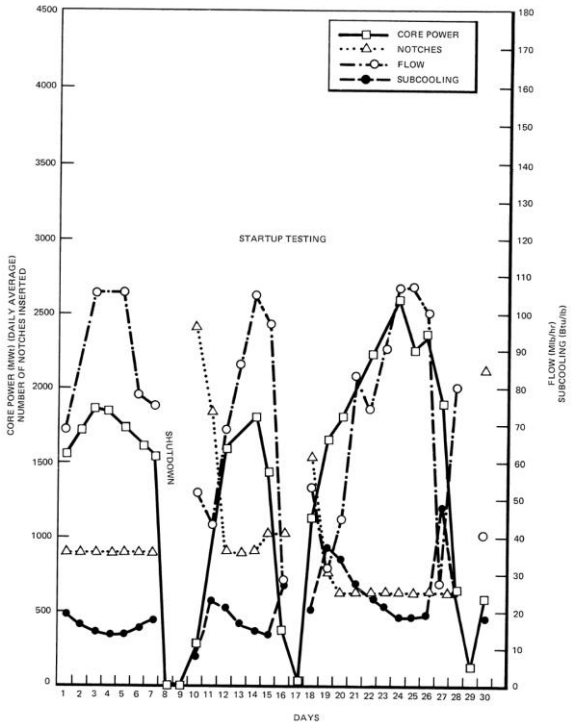
BWR :: Peach Bottom 2 Cycles 1-3

Table 3.10 PB2 cycle 1 core data

Total fuel assemblies	764
Control elements	185
Average linear heat rate, kw/ft	7.037
Rated core thermal power (MW)	3293
Active fuel length, cm (ft)	365.76 (12)
Core lattice pitch, cm (in)	30.48 (12.0)
Water/UO_2 ratio (Cold)	2.51
Total weight of U in core (ST)	159.2
Number of in-core flux monitors	43



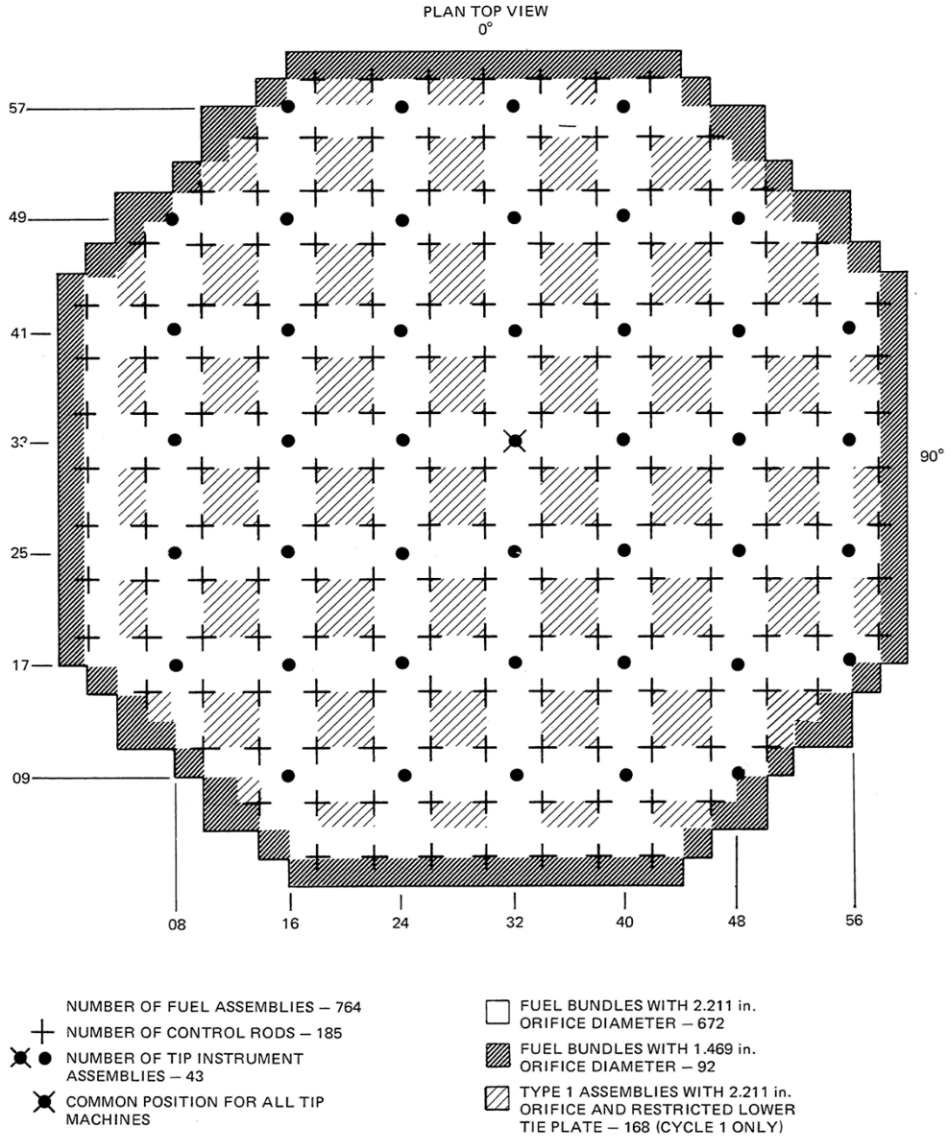


Figure 3.15 Core orificing and TIP system arrangement in PB2

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BWR :: Peach Bottom 2 Cycles 1-3

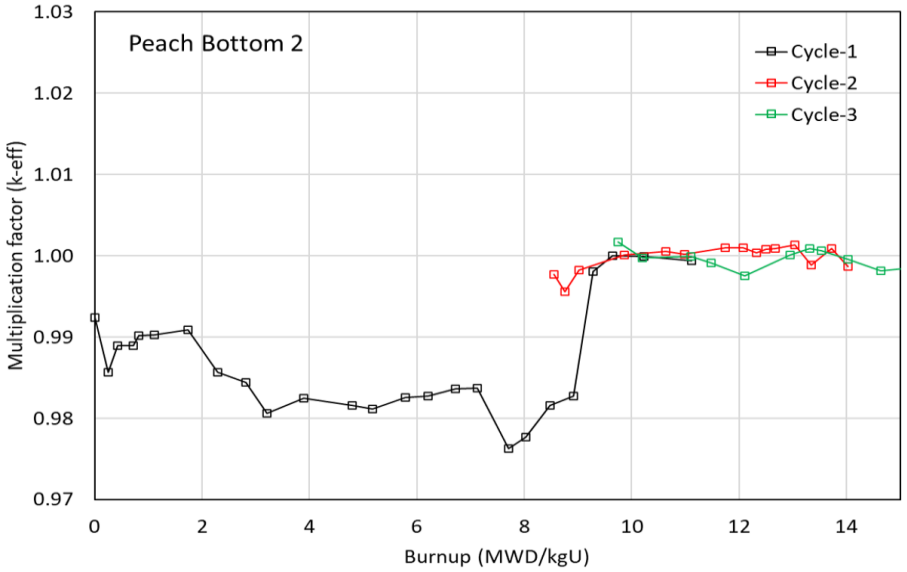


Figure 3.17 Calculated core reactivities of the PB2 cycles 1−3 at operating conditions

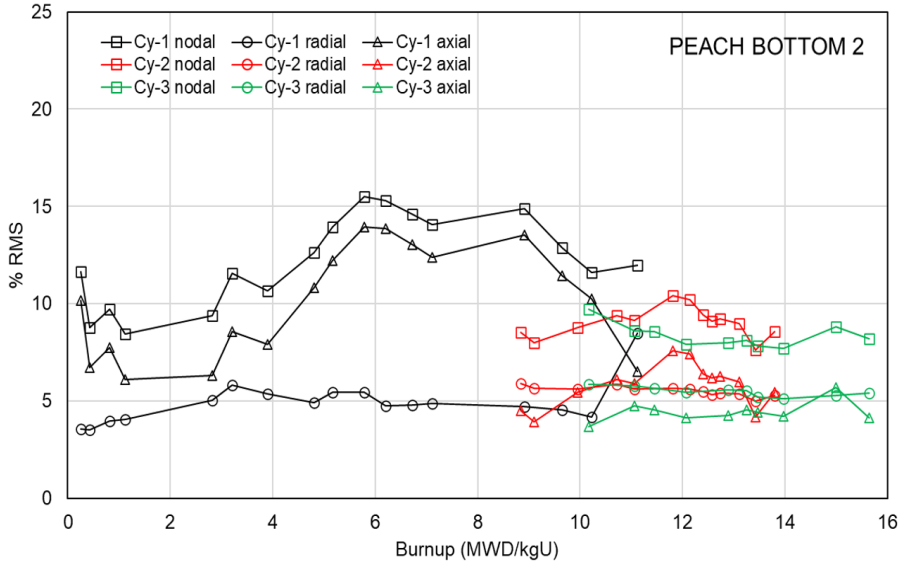
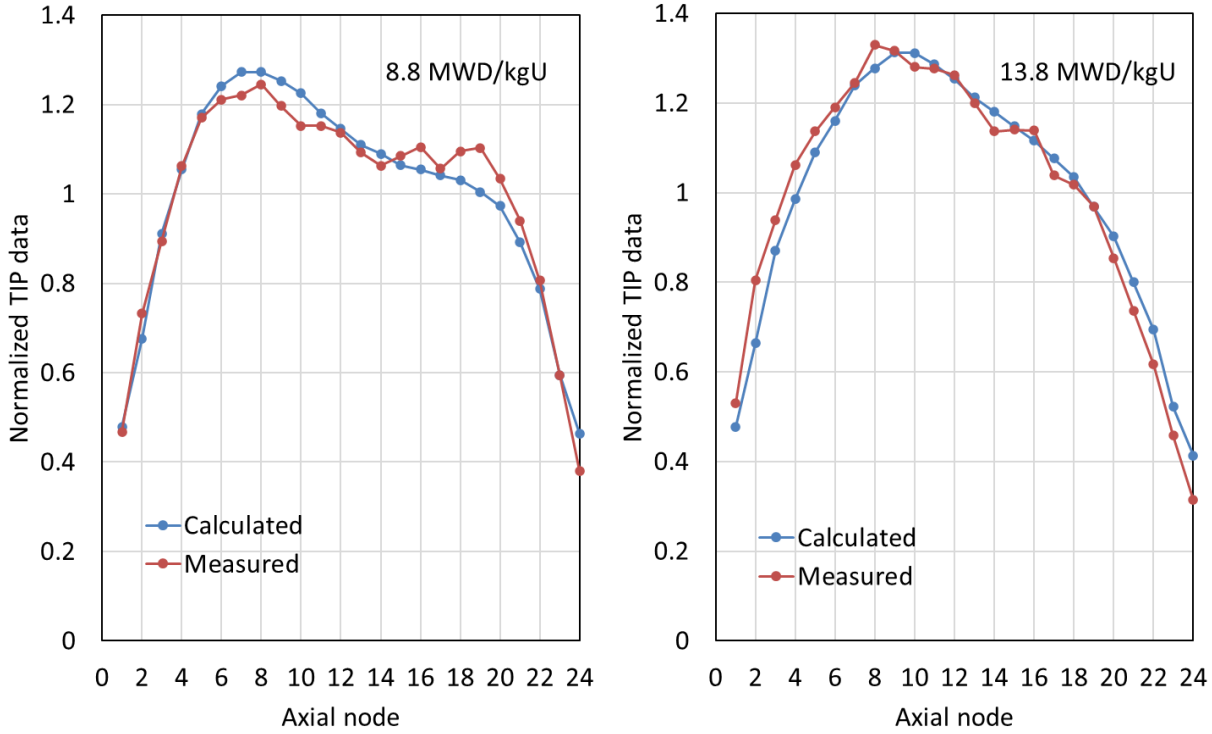


Figure 3.18 RMS errors between the measured and calculated TIP data in PB2



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BWR :: Hatch 1 Cycles 1-3

Table 3.12 Hatch 1 cycle 1 core data

Total fuel assemblies	560
Control elements	136
Rate core thermal power (MW)	2436
Active fuel length, cm (ft)	365.76 (12)
Core lattice pitch, cm (in)	30.48 (12.0)
Water/UO2 Ratio (Cold)	2.53
Total weight of U in core (ST)	119.1
Number of in-core flux monitors	31

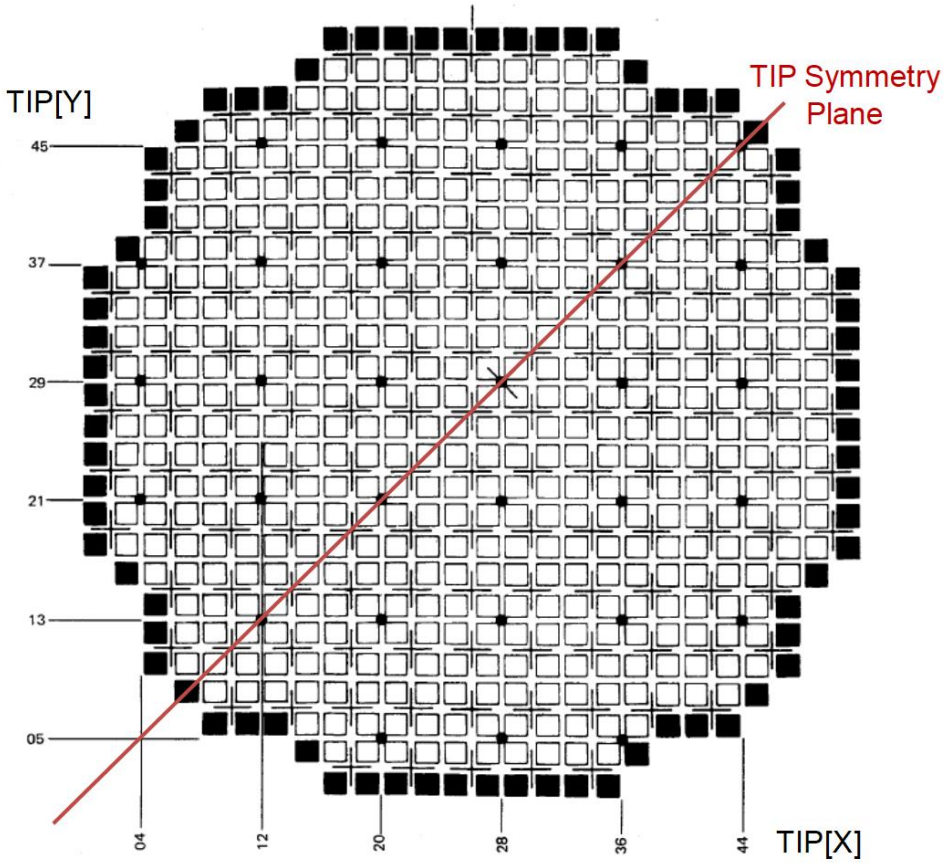

Figure 3.19 Illustration of TIP Symmetry Plane in Hatch 1

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BWR :: Hatch 1 Cycles 1-3

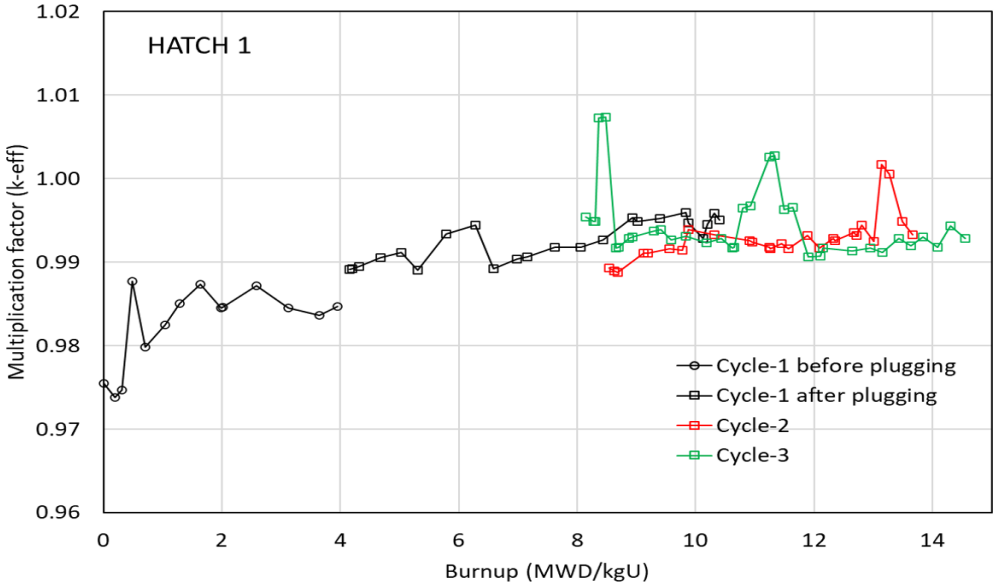


Figure 3.20 Calculated core reactivities of the Hatch 1 cycles 1–3 at operating conditions

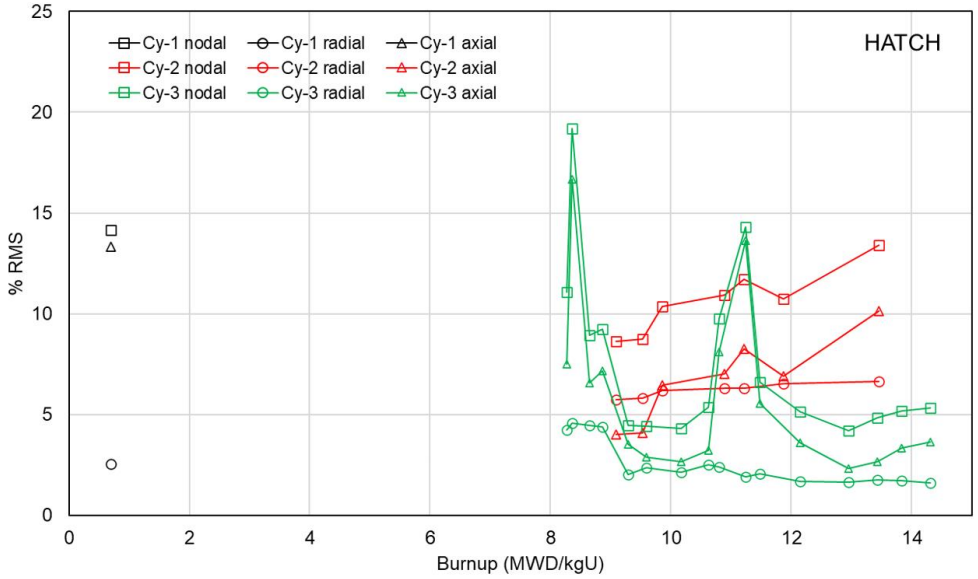
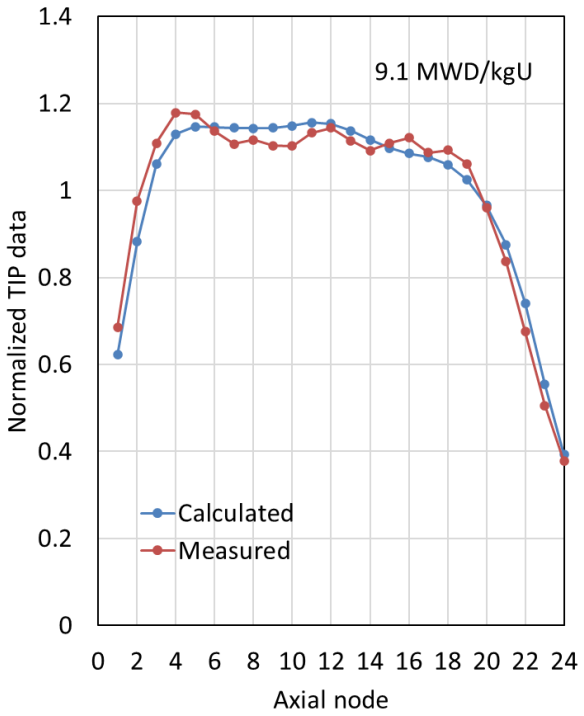
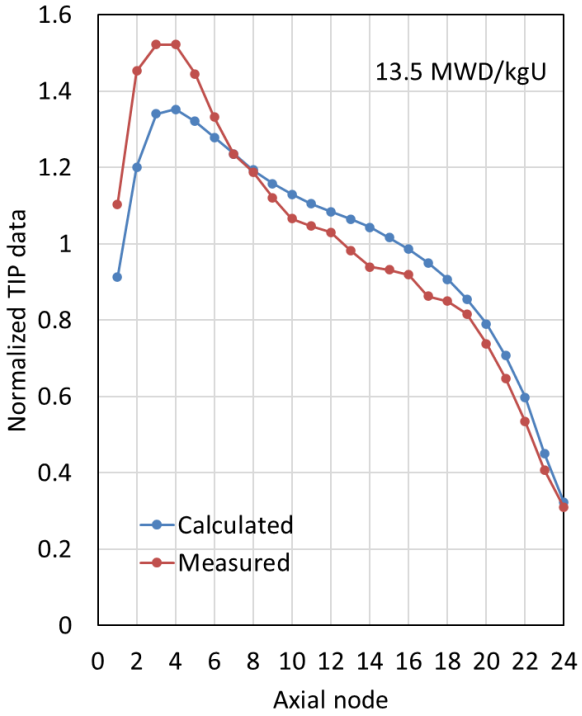


Figure 3.21 RMS errors between the measured and calculated TIP data in Hatch 1





Discussion I

- **Pending issues in Polaris**
  - Gamma smeared power form factors

- **Pending issues in PARCS**
  - Instability of reload cycle calculation
    - Unnecessary independent HZP fuel shuffling PARCS inputs
    - Weird HZP results for reload cycles
    - ← Need to have these issues resolved in Q3
  - Limitation in the capability of discharging burnable poisons after cycle
    - Tried to use non-BP cross sections, but the result is weird
    - Micro depletion capability may resolve this issue
    - ← Need to have this issue resolved in Q3
  - No assembly rotation capability with quadrant dependent cross section sets
    - 4-node capability in an assembly
    - ← Need to have this issue resolved in Q3
  - Too many branch cases
    - ← Not urgent, but may need to have this issue resolved in Q3

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Discussion II

- **More plants and more cycles**
  - Require more than 20 cycles for each reactor type
- **Candidate PWRs and BWRs**

Type	Reactors	# of cycles	Remark
PWR	San Onofre Nuclear Generating Station (SONGS) Unit 1	6	
	San Onofre Nuclear Generating Station (SONGS) Unit 2	5	
	San Onofre Nuclear Generating Station (SONGS) Unit 3	4	
	Arkansas Nuclear One Unit 2 (ANO-2)		
	Three Mile Island (TMI) Unit 1		
	SURRY Unit 1	3	
	Watt Bar Nuclear Plant Unit 1	9	Cycles 4-12
	Watt Bar Nuclear Plant Unit 2	2	
	Duke Power McGuire Units 1 and 2		
	Duke Power Catawba Units 1 and 2		
	Westinghouse AP1000		Gen3+
	KHNP APR1400		Gen3+
BWR	Quad Cities	3	
	Peach Bottom Unit 3	6	Cycles 17-22
	Limerick	5	Cycles 13-15
	Needs more BWR plants		

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Conclusion

- **This is on-going project.**
  - Final goal is to complete the following table for uncertainties.

Table 6.1 Uncertainties for the key nuclear parameters of PWR and BWR

PWR		BWR	
Parameter	Uncertainty	Parameter	Uncertainty
Core reactivity (pcm)		Core reactivity (pcm)	
Inverse boron worth (ppm/pcm)			
Temperature coefficient (pcm/F) - Isothermal - Moderator - Fuel			
Control rod worth (%) - Total - Individual			
Pin-to-box factor (%)	2.0 (1.53)	Pin-to-box factor	2.0 (1.53)
Assembly peaking (%) - F_q - F_{xy} - F_r		Assembly peaking (%) - F_q - F_{xy} - F_r	
Pin peaking (%) - F_q - F_{xy} - F_r, $F_{\Delta H}$		Pin peaking (%) - F_q - F_{xy} - F_r, $F_{\Delta H}$	

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On-going and Future Works

- **Calculation notes**
  - Detailed information for the Polaris and PARCS input preparation and input/output files
    - Polaris validation through critical experiment benchmarks
    - BEAVRS (reference format by Kim), WBN1, PB2, Hatch1
  - Flux map and TIP comparison
    - Fortran → Python: One program
    - Graphical comparison
- **Repository**
  - Standard format for the measured data and database
  - Update repository
- **Additional benchmark calculations**
  - PWR
    - SURRY: 3 cycles
    - Turkey Point: 3 cycles
    - SONGS Units 1, 2 and 3: 15 cycles
  - BWR
    - Quad Cities: 3 cycles
    - Monticello: 3 cycles

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On-going and Future Works

- **Micro Nodal Capability**
  - Polaris-GenPMAXS-PARCS micro nodal capability
    - GenPMAXS and PARCS are almost ready
    - Polaris is under improvement
- **Enhance cross section functionalization**
  - Implement the Nuclear Vendor type approach
    - Implementation in Q2 and test in Q3
- **Verification for reflector XS generation and Enhancement**
  - Polaris-PARCS vs. VERA vs. CE-KENO
    - 2D core

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ACKNOWLEDGEMENT

This investigation was supported by US Nuclear Regulatory Commission.