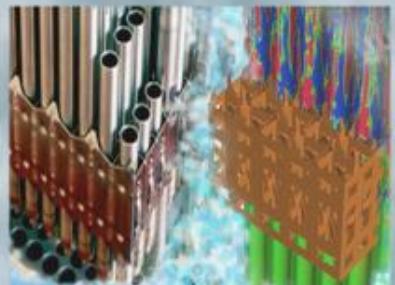
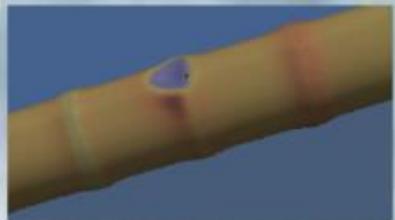
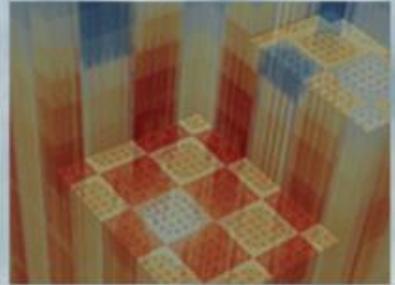


Specification for the VERA Depletion Benchmark Suite

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Kang Seog Kim



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EXECUTIVE SUMMARY

The CASL neutronics simulator MPACT is under development for the neutronics and T-H coupled simulation for the pressurized water reactor. MPACT includes the ORIGEN-API and internal depletion module to perform depletion calculations based upon neutron-material reaction and radioactive decay. It is a challenge to validate the depletion capability because of the insufficient measured data. One of the detoured methods to validate it is to perform a code-to-code comparison for benchmark problems. In this study a depletion benchmark suite has been developed and a detailed guideline has been provided to obtain meaningful computational outcomes which can be used in the validation of the MPACT depletion capability.

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ACRONYMS

2D	Two-Dimensional
CASL	Consortium for Advanced Simulation of Light Water Reactors
FPY	Fission Product Yield
MOC	Method of Characteristics
MG	Multi-group (as in cross sections)
ORNL	Oak Ridge National Laboratory
PND	Particle (Atomic) Number Density
PWR	Pressurized water reactor
T-H	Thermal Hydraulic
UM	University of Michigan
VERA	Virtual Environment for Reactor Applications

1. INTRODUCTION

The CASL neutronics simulator MPACT is under development for the neutronics and T-H coupled simulation for the pressurized water reactor. MPACT includes the ORIGEN-API and internal depletion module to perform depletion calculations based upon neutron-material reaction and radioactive decay. It is a challenge to validate the depletion capability because of the insufficient measured data. One of the detoured methods to validate it is to perform a code-to-code comparison for depletion benchmark problems. In this study a depletion benchmark suite has been developed and a detailed guideline has been provided to obtain meaningful computational outcomes which can be used in the validation of the MPACT depletion capability.

The benchmark problems have been developed based on “The VERA Core Physics Benchmark Progression Problems” [God14]. This document provides the detailed design data and guide lines to obtain meaningful and valuable outcomes for the validation of the MPACT depletion capability.

- Geometry and composition data required in preparing user input files for the engaged simulation codes in Chapter 2,
- Recoverable energies per fission to exclude a difference of neutron flux level due to code specific recoverable energies per fission in Chapter 3,
- Burnup chains of the ORIGEN-API to figure out the differences of burnup chains with the engaged simulation programs in Chapter 4,
- Detailed description for the benchmark problems, user options and nuclear parameters to be edited and compared in Chapter 5.

2. GEOMETRY AND MATERIAL DATA

The depletion benchmark problems have been developed based on the VERA progression problems [God14]. Table 2.1 provides the geometrical and material data for the benchmark problems which come from the VERA progression problems #1 and #2.

Table 2.2 provides density and atomic number densities for each material which should be utilized in depletion calculation to exclude a bias due to the difference in initial atomic number densities.

Table 2.1 Geometry and material data (1/2)

Material	Parameter	Value	Remark
Core	Pressure (bar)	155.13	2250 psia
	Power Density (w/gU)	40.00	
	Fuel assembly power (MW)/cm	0.050324728	Variable
	Assembly Pitch (cm)	21.5000	
	Pin Pitch (cm)	1.2600	
Fuel	Pellet Radius (cm)	0.4096	
	Material	UO ₂	Various ²³⁵ U w/o
	Density (g/cm ³)	10.2570	
Gadolinia Rod	Pellet Radius (cm)	0.4096	
	Material	UO ₂ +Gd ₂ O ₃	1.8w/o ²³⁵ U, 5% Gd ₂ O ₃
	Density (g/cm ³)	10.1110	
Clad	Inner Radius (cm)	0.4180	
	Outer Radius (cm)	0.4750	
	Material	Zircaloy-4	
	Density (g/cm ³)	6.5600	
Guide Tube	Inner Radius (cm)	0.5610	
	Outer Radius (cm)	0.6020	
	Material	Zircaloy-4	
	Density (g/cm ³)	6.5600	
Instrumentation Tube	Inner Radius (cm)	0.5590	
	Outer Radius (cm)	0.6050	
	Material	Zircaloy-4	
	Density (g/cm ³)	6.5600	
Thimble inside Instrumentation Tube	Inner Radius of thimble (cm)	0.2580	
	Outer Radius of thimble (cm)	0.3820	
	Material	SS304	
	Internal material	⁴ He	
	Material between thimble and IT	Moderator	

Table 2.1 Geometrical and material data (2/2)

Material	Parameter	Value	Remark
Control Rod (AgInCd & B ₄ C)	AgInCd Radius (cm)	0.3820	
	AgInCd Density (g/cm ³)	10.2000	
	B ₄ C Radius (cm)	0.3730	
	B ₄ C Density (g/cm ³)	1.7600	
	Clad Inner Radius (cm)	0.3860	
	Clad Outer Radius (cm)	0.4840	
	SS304 Clad Density (g/cm ³)	7.8000	
IFBA	Coating Thickness (μm)	10.0000	
	Material	ZrB ₂	
	¹⁰ B enrichment (w/o)	50.0	
	Density (g/cm ³)	3.8500	
WABA	Material	B ₄ C+Al ₂ O ₃	
	Density (g/cm ³)	3.6500	
	Inner Clad Inner Radius (cm)	0.2860	
	Inner Clad Outer Radius (cm)	0.3390	
	Inner/Outer Clad Material	Zircaloy-4	
	Poison Inner Radius (cm)	0.3530	
	Poison Outer Radius (cm)	0.4040	
	Outer Clad Inner Radius (cm)	0.4180	
	Outer Clad Outer Radius (cm)	0.4840	
Pyrex	Material	B ₂ O ₃ +SiO ₂	12.5 w/o B ₂ O ₃
	Density (g/cm ³)	2.2500	
	Inner Clad Inner Radius (cm)	0.2140	
	Inner Clad Outer Radius (cm)	0.2310	
	Inner/Outer Clad Material	SS-304	
	Poison Inner Radius (cm)	0.2410	
	Poison Outer Radius (cm)	0.4270	
	Outer Clad Inner Radius (cm)	0.4370	
	Outer Clad Outer Radius (cm)	0.4840	

Table 2.2 Density and atomic number density for each material (1/2)

Material	Density(g/cm ³)	Isotope ID	PND (/barn-cm)	Isotope ID	PND (/barn-cm)
Fuel (2.1%)	10.257	92234	4.02487E-06	92238	2.23868E-02
		92235	4.86484E-04	8016	4.57590E-02
		92236	2.23756E-06		
Fuel (3.1%)	10.257	92234	6.11864E-06	92238	2.21546E-02
		92235	7.18132E-04	8016	4.57642E-02
		92236	3.29861E-06		
Fuel (3.6%)	10.257	92234	7.21203E-06	92238	2.20384E-02
		92235	8.33952E-04	8016	4.57669E-02
		92236	3.82913E-06		
Fuel (4.6%)	10.257	92234	9.39876E-06	92238	2.18062E-02
		92235	1.06559E-03	8016	4.57721E-02
		92236	4.89014E-06		
Gap	1.79E-04	2004	2.68714E-05		
Cladding (Zirc-4)	6.56	40090	2.18865E-02	26054	8.68307E-06
		40091	4.77292E-03	26056	1.36306E-04
		40092	7.29551E-03	26057	3.14789E-06
		40094	7.39335E-03	26058	4.18926E-07
		40096	1.19110E-03	24050	3.30121E-06
		50112	4.68066E-06	24052	6.36606E-05
		50114	3.18478E-06	24053	7.21860E-06
		50115	1.64064E-06	24054	1.79686E-06
		50116	7.01616E-05	72174	3.54138E-09
		50117	3.70592E-05	72176	1.16423E-07
		50118	1.16872E-04	72177	4.11686E-07
		50119	4.14504E-05	72178	6.03806E-07
		50120	1.57212E-04	72179	3.01460E-07
		50122	2.23417E-05	72180	7.76449E-07
		50124	2.79392E-05		
Moderator 565 K 1300 ppm	0.743	8016	2.48112E-02	5010	1.07070E-05
		1001	4.96224E-02	5011	4.30971E-05
Moderator 600 K 1300 ppm	0.700	8016	2.33753E-02	5010	1.00874E-05
		1001	4.67505E-02	5011	4.06030E-05
IFBA	3.85	5010	2.16410E-02	40092	3.54348E-03
		5011	1.96824E-02	40094	3.59100E-03
		40090	1.06304E-02	40096	5.78528E-04
		40091	2.31824E-03		
Pyrex	2.25	5010	9.63266E-04	14028	1.81980E-02
		5011	3.90172E-03	14029	9.24474E-04
		8016	4.67761E-02	14030	6.10133E-04
Gadolinia 5% Gd ₂ O ₃ 95% UO ₂ 1.8% ²³⁵ U Fuel	10.111	92234	3.18096E-06	64155	2.48606E-04
		92235	3.90500E-04	64156	3.43849E-04
		92236	1.79300E-06	64157	2.62884E-04
		92238	2.10299E-02	64158	4.17255E-04
		64152	3.35960E-06	64160	3.67198E-04
		64154	3.66190E-05	8016	4.53705E-02

Table 2.2 Density and atomic number density for each material (2/2)

Material	Density(g/cm ³)	Isotope ID	PND (/barn-cm)	Isotope ID	PND (/barn-cm)
SS304	7.8	6000	3.20895E-04	26054	3.44776E-03
		14028	1.58197E-03	26056	5.41225E-02
		14029	8.03653E-05	26057	1.24992E-03
		14030	5.30394E-05	26058	1.66342E-04
		15031	6.99938E-05	28058	5.30854E-03
		24050	7.64915E-04	28060	2.04484E-03
		24052	1.47506E-02	28061	8.88879E-05
		24053	1.67260E-03	28062	2.83413E-04
		24054	4.16346E-04	28064	7.21770E-05
		25055	1.75387E-03		
AgInCd	10.2	47107	2.36159E-02	48112	6.59276E-04
		47109	2.19403E-02	48113	3.33873E-04
		48106	3.41523E-05	48114	7.84957E-04
		48108	2.43165E-05	48116	2.04641E-04
		48110	3.41250E-04	49113	3.44262E-04
		48111	3.49720E-04	49115	7.68050E-03
B ₄ C	1.76	5010	1.52689E-02	6000	1.91820E-02
		5011	6.14591E-02		
WABA B ₄ C-Al ₂ O ₃	3.65	5010	2.98553E-03	8016	5.85563E-02
		5011	1.21192E-02	13027	3.90223E-02
		6000	3.77001E-03		

3. RECOVERABLE ENERGY PER FISSION

The neutron flux level would impact on predicting isotopic inventories at burnup calculation which is estimated by using the code specific recoverable energies per fission. Therefore, it is recommended to utilize the common recoverable energy per fission provided in Table 3.1.

Table 3.1 Recoverable energy per fission

No	ID	Nuclide	ENDF/B-7.0		ENDF/B-7.1	
			Kappa(w-s)	Kappa0(w-s)	Kappa(w-s)	Kappa0(w-s)
1	90230	^{230}Th	3.24352E-11	3.05372E-11	3.22841E-11	2.89031E-11
2	90232	^{232}Th	3.22345E-11	3.01965E-11	3.22345E-11	3.01965E-11
3	91231	^{231}Pa	3.38655E-11	3.06082E-11	3.38655E-11	2.97356E-11
4	91233	^{233}Pa	3.27020E-11	3.06082E-11	3.26046E-11	2.97452E-11
5	92232	^{232}U	3.40754E-11	3.06082E-11	3.40754E-11	2.95739E-11
6	92233	^{233}U	3.20712E-11	3.06082E-11	3.20712E-11	3.06082E-11
7	92234	^{234}U	3.26494E-11	3.07364E-11	3.26494E-11	3.07364E-11
8	92235	^{235}U	3.24187E-11	3.09997E-11	3.24187E-11	3.09872E-11
9	92236	^{236}U	3.30019E-11	3.11610E-11	3.30019E-11	3.11610E-11
10	92237	^{237}U	3.36652E-11	3.14446E-11	3.36652E-11	3.00925E-11
11	92238	^{238}U	3.40626E-11	3.17285E-11	3.40626E-11	3.16891E-11
12	92240	^{240}U	3.33592E-11	3.17330E-11	3.33592E-11	3.17330E-11
13	93237	^{237}Np	3.37405E-11	3.14622E-11	3.37405E-11	3.14622E-11
14	93238	^{238}Np	3.37181E-11	3.18579E-11	3.37181E-11	3.19722E-11
15	93239	^{239}Np	3.42660E-11	3.18579E-11	3.42660E-11	3.04126E-11
16	94236	^{236}Pu	3.29971E-11	3.11610E-11	3.34433E-11	3.19691E-11
17	94237	^{237}Pu	3.30131E-11	3.13869E-11	3.38885E-11	3.22623E-11
18	94238	^{238}Pu	3.36748E-11	3.16240E-11	3.41258E-11	3.21010E-11
19	94239	^{239}Pu	3.43312E-11	3.18586E-11	3.43312E-11	3.18679E-11
20	94240	^{240}Pu	3.43157E-11	3.19589E-11	3.43157E-11	3.19589E-11
21	94241	^{241}Pu	3.47426E-11	3.23611E-11	3.47426E-11	3.23611E-11
22	94242	^{242}Pu	3.47643E-11	3.22969E-11	3.49302E-11	3.24889E-11
23	94244	^{244}Pu	3.41266E-11	3.25004E-11	3.35567E-11	3.19305E-11
24	95241	^{241}Am	3.48348E-11	3.23578E-11	3.48348E-11	3.23578E-11
25	95242	^{242}Am	3.45085E-11	3.22969E-11	3.51714E-11	3.29599E-11
26	95243	^{243}Am	3.56147E-11	3.26238E-11	3.56147E-11	3.26238E-11
27	95242m	$^{242\text{m}}\text{Am}$	3.56147E-11	3.26238E-11	3.56147E-11	3.26238E-11
28	96241	^{241}Cm	3.40465E-11	3.24203E-11	3.51880E-11	3.35618E-11
29	96242	^{242}Cm	3.54821E-11	3.24524E-11	3.54821E-11	3.25983E-11
30	96243	^{243}Cm	3.50159E-11	3.24764E-11	3.50159E-11	3.26885E-11
31	96244	^{244}Cm	3.54308E-11	3.25004E-11	3.54308E-11	3.33858E-11
32	96245	^{245}Cm	3.45048E-11	3.27359E-11	3.45060E-11	3.28798E-11
33	96246	^{246}Cm	3.51248E-11	3.29731E-11	3.54721E-11	3.37309E-11
34	96247	^{247}Cm	3.48348E-11	3.32086E-11	3.51698E-11	3.35436E-11
35	96248	^{248}Cm	3.50703E-11	3.34441E-11	3.55936E-11	3.39674E-11
36	97249	^{249}Bk	3.50703E-11	3.34441E-11	3.60559E-11	3.44297E-11
37	98249	^{249}Cf	3.50703E-11	3.34441E-11	3.55494E-11	3.39232E-11
38	98250	^{250}Cf	3.50703E-11	3.34441E-11	3.68134E-11	3.51872E-11
39	98251	^{251}Cf	3.50703E-11	3.34441E-11	3.58147E-11	3.41885E-11
40	98252	^{252}Cf	3.50703E-11	3.34441E-11	3.68984E-11	3.52721E-11

4. BURNUP CHAIN

Typically deterministic/Monte Carlo programs include their own burnup chains and libraries. The SCALE-ORIGEN and CASL-ORIEGN include two different burnup chains which are full and simplified ones. The simplified burnup chain has been developed to include 255 nuclides and to have very good agreement with the full burnup chain especially for the multiplication factor. Since the latest SCALE-ORIGEN burnup chains and libraries reflect the most up-to-date data and methodology, it is recommended to utilize the ORIGEN-API burnup chains and libraries for benchmark calculations. The SCALE-ORIGEN libraries will be provided upon request for which the SCALE license should be acquired at first. If the program is not ready yet to handle the SCALE-ORIGEN libraries, it is required to include its own burnup chain and libraries in the report.

Appendices A and B provide constituent 255 nuclides for the simplified burnup chain and each column includes the following indicators.

- CAT: Category of nuclides
 - 1 : Activation nuclides
 - 2 : Heavy metal nuclides
 - 3 : Fission product nuclides
- ID: Numeric nuclide ID in ORIGEN = ZZZAAAI
 - ZZZ : Atomic number
 - AAA : Atomic mass number
 - I : Stable or meta-stable (0: stable; 1: meta)
- IFPY: Indicator for fission product yield
 - 0 : Non FPY
 - 1 : Direct FPY
 - 2 : Cumulative FPY
 - 3 : Special treatment with weight fractions (W_i)

5. DEPLETION BENCHMARK PROBLEMS

5.1 Benchmark problems

The depletion benchmark suite includes 9 single pin and 16 fuel assembly problems with various fuel temperatures, ^{235}U enrichments, control rods and burnable poisons as shown in Table 5.1. The pin configurations of fuel rods, guide/instrument tubes and burnable poisons are shown in Figure 5.1. The geometrical and material data for the benchmark problems are provided in Chapter 2. In order to verify the input data prepared by participant Table 5.2 provides the multiplication factors obtained by KENO-CE with ENDF/B-7.0 at 0.0 MWD/kgU.

Table 5.1 Single pin and assembly depletion benchmark problems

Problem	Description	Temperature (K)			Moderator Density	^{235}U w/o	Power density (w/gU)
		Moderator	Clad	Fuel			
1A	Pin 3.1w/o $T_F=565\text{K}$	565	565	565	0.743	3.1	40.0
1B	Pin 3.1w/o $T_F=600\text{K}$	600	600	600	0.700	3.1	40.0
1C	Pin 3.1w/o $T_F=900\text{K}$	600	600	900	0.700	3.1	40.0
1D	Pin 3.1w/o $T_F=1200\text{K}$	600	600	1200	0.700	3.1	40.0
1E	Pin IFBA 3.1w/o $T_F=600\text{K}$	600	600	900	0.700	3.1	40.0
1F	Pin 2.1w/o $T_F=900\text{K}$	600	600	900	0.700	2.1	40.0
1G	Pin 3.6w/o $T_F=900\text{K}$	600	600	900	0.700	3.6	40.0
1H	Pin 4.6w/o $T_F=900\text{K}$	600	600	900	0.700	4.6	40.0
1I	Pin Gadolinia rod (5% Gd_2O_3)	600	600	900	0.700	1.8	40.0
1J	Pin 3.1w/o $T_F=600/900/1200\text{K}$	600	600	600/900/1200	0.700	3.1	40.0
2A	FA No Poisons $T_F=565\text{K}$	565	565	565	0.743	3.1	40.0
2B	FA No Poisons $T_F=600\text{K}$	600	600	600	0.700	3.1	40.0
2C	FA No Poisons $T_F=900\text{K}$	600	600	900	0.700	3.1	40.0
2D	FA No Poisons $T_F=1200\text{K}$	600	600	1200	0.700	3.1	40.0
2E	FA 12 Pyrex	600	600	900	0.700	3.1	40.0
2F	FA 24 Pyrex	600	600	900	0.700	3.1	40.0
2G	FA 24 AIC	600	600	900	0.700	3.1	40.0
2H	FA 24 B4C	600	600	900	0.700	3.1	40.0
2I	FA Instrument Thimble	600	600	900	0.700	3.1	40.0
2J	FA Instrument + 24 Pyrex	600	600	900	0.700	3.1	40.0
2K	FA Zoned + 24 Pyrex	600	600	900	0.700	3.1/3.6	40.0
2L	FA 80 IFBA	600	600	900	0.700	3.1	40.0
2M	FA 128 IFBA	600	600	900	0.700	3.1	40.0
2N	FA 104 IFBA + 20 WABA	600	600	900	0.700	3.1	40.0
2O	FA 12 Gadolinia	600	600	900	0.700	3.1/1.8	40.0
2P	FA 24 Gadolinia	600	600	900	0.700	3.1/1.8	40.0

Table 5.2 Multiplication factors at 0.0 MWD/kgU burnup

Problem	Description	Temperature (K)			KENO-CE k_{eff}
		Moderator	Clad	Fuel	
1A	Pin 3.1w/o $T_F=565K$	565	565	565	1.18704 ± 0.00005
1B	Pin 3.1w/o $T_F=600K$	600	600	600	1.18428 ± 0.00017
1C	Pin 3.1w/o $T_F=900K$	600	600	900	1.17393 ± 0.00016
1D	Pin 3.1w/o $T_F=1200K$	600	600	1200	1.16516 ± 0.00013
1E	Pin IFBA 3.1w/o $T_F=600K$	600	600	900	0.76521 ± 0.00022
1F	Pin 2.1w/o $T_F=900K$	600	600	900	1.05835 ± 0.00017
1G	Pin 3.6w/o $T_F=900K$	600	600	900	1.21335 ± 0.00018
1H	Pin 4.6w/o $T_F=900K$	600	600	900	1.27094 ± 0.00018
1I	Pin Gadolinia rod (5% Gd_2O_3)	600	600	900	0.21820 ± 0.00010
1J	Pin 3.1w/o $T_F=600/900/1200K$	600	600	600/900/1200	1.17451 ± 0.00014
2A	FA No Poisons $T_F=565K$	565	565	565	1.18218 ± 0.00002
2B	FA No Poisons $T_F=600K$	600	600	600	1.18240 ± 0.00012
2C	FA No Poisons $T_F=900K$	600	600	900	1.17354 ± 0.00014
2D	FA No Poisons $T_F=1200K$	600	600	1200	1.16543 ± 0.00015
2E	FA 12 Pyrex	600	600	900	1.06072 ± 0.00016
2F	FA 24 Pyrex	600	600	900	0.96541 ± 0.00017
2G	FA 24 AIC	600	600	900	0.83443 ± 0.00017
2H	FA 24 B4C	600	600	900	0.77337 ± 0.00021
2I	FA Instrument Thimble	600	600	900	1.17256 ± 0.00012
2J	FA Instrument + 24 Pyrex	600	600	900	0.96476 ± 0.00017
2K	FA Zoned + 24 Pyrex	600	600	900	1.00886 ± 0.00019
2L	FA 80 IFBA	600	600	900	1.01133 ± 0.00018
2M	FA 128 IFBA	600	600	900	0.93205 ± 0.00017
2N	FA 104 IFBA + 20 WABA	600	600	900	0.86123 ± 0.00020
2O	FA 12 Gadolinia	600	600	900	1.04004 ± 0.00017
2P	FA 24 Gadolinia	600	600	900	0.91993 ± 0.00016

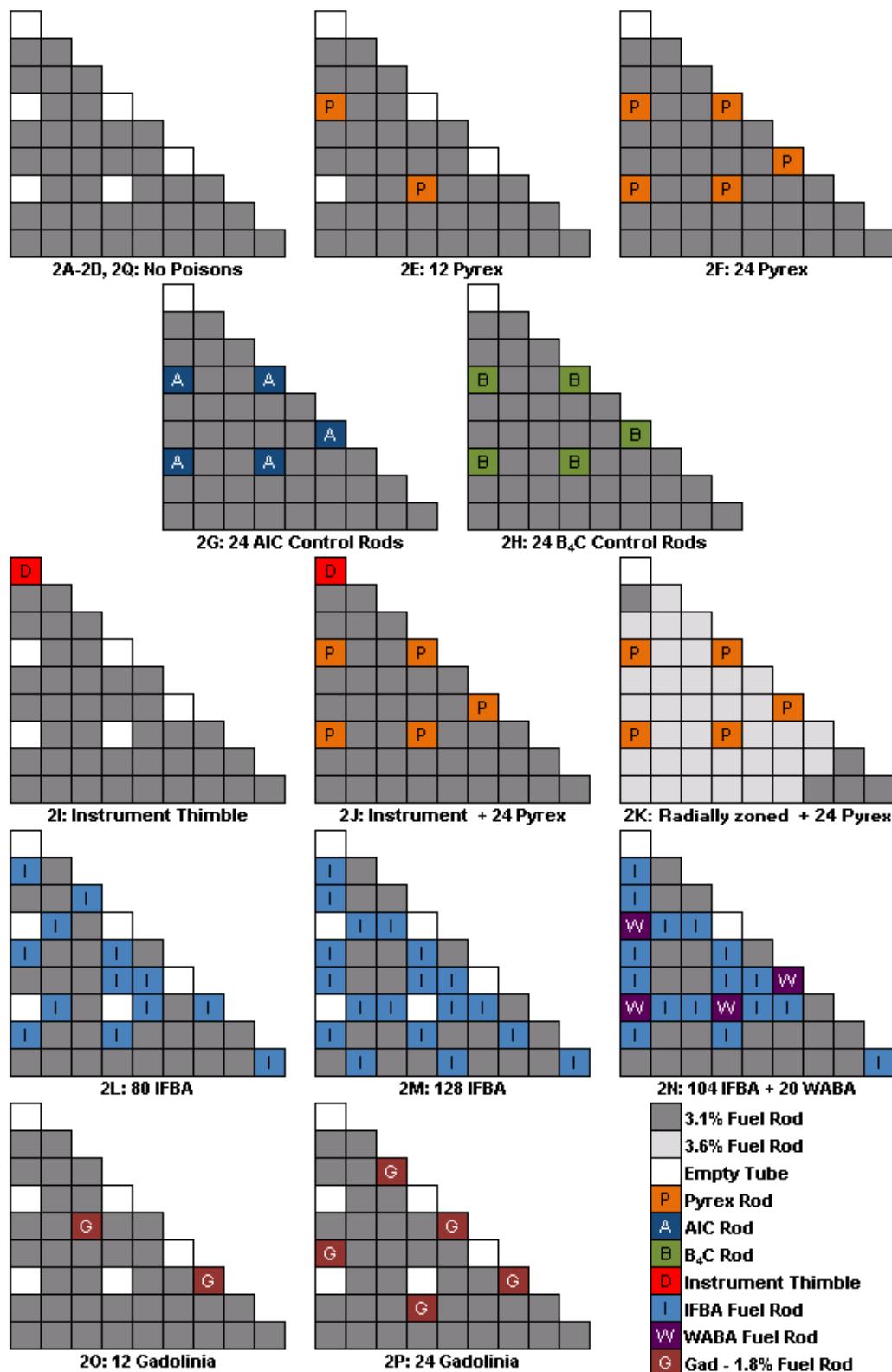


Figure 5.1 Lattice pin cell configuration

5.2 Calculation options

The computational results of the depletion calculations would be dependent upon user options and libraries. Therefore, in order not to have any difference due to the differences of user option and library the following user options and library should be utilized in the calculations.

- Xenon option
 - Non-equilibrium for all cases
 - Equilibrium for the specified cases in Table 5.4 (**1C** and **2C**)
- Power density
 - Table 5.1 provides the specific power density for each case (40.0 w/gU).
- Burnup points
 - Table 5.3 provides the burnup points.
- Library
 - ENDF/B-7.0 or ENDF/B-7.1 (7.0 is more recommended.)
- The number of depletion zones
 - UO₂ pellet: 3 equi-volumetric zones
 - UO₂+Gd₂O₃ Gadolinia rod: 5 equi-volumetric zones
 - WABA & PYREX: 3 equi-volumetric zones

Table 5.3 Burnup points and editing options

Step	Burnup			Edit			Step	Burnup			Edit		
	MWD/kgU	EFPD	P.D.	R.R.	Flux	MWD/kgU		EFPD	P.D.	R.R.	Flux		
1	0.00	0.00	O	O	O	21	17.00	425.00					
2	0.01	0.25				22	18.00	450.00					
3	0.25	6.25				23	19.00	475.00					
4	0.50	12.50				24	20.00	500.00	O	O	O		
5	1.00	25.00				25	22.50	562.50					
6	2.00	50.00				26	25.00	625.00					
7	3.00	75.00				27	27.50	687.50					
8	4.00	100.00				28	30.00	750.00	O	O	O		
9	5.00	125.00	O	O	O	29	32.50	812.50					
10	6.00	150.00				30	35.00	875.00					
11	7.00	175.00				31	37.50	937.50					
12	8.00	200.00				32	40.00	1000.00	O	O	O		
13	9.00	225.00				33	42.50	1062.50					
14	10.00	250.00	O	O	O	34	45.00	1125.00					
15	11.00	275.00				35	47.50	1187.50					
16	12.00	300.00				36	50.00	1250.00	O	O	O		
17	13.00	325.00				37	52.50	1312.50					
18	14.00	350.00				38	55.00	1375.00					
19	15.00	375.00	O	O	O	39	57.50	1437.50					
20	16.00	400.00				40	60.00	1500.00					

P.D. : Power Distribution

R.R. : Reaction Rate

5.3 Edition of reactor physics parameters

In order to complete the code-to-code comparison the following parameters need to be edited which are also provided in Table 5.3.

- Multiplication factors (keff) vs. burnup
 - All cases
 - All burnup points
- Pin power distribution
 - For the problems: **2C, 2F, 2N** and **2P**
 - For the burnup points: 1, 8, 13, 18, 23, 27, 31 and 35
- Particle(atomic) number densities (PND)
 - For the problems: **1C, 1E** and **1H**
 - PND should be edited for each depletion zone. (e.g. UO₂ pellet=3 zones)
 - PND needs to be edited for the nuclides in Table 4.1.
 - All burnup points
- Multigroup scalar fluxes
 - For the problems: **1C** and **1H**
 - For the burnup points: 1, 8, 13, 18, 23, 27, 31 and 35
 - Power scaled 1-group scalar flux for each depletion zone
 - Monte Carlo codes: Multi-group (47-group) normalized scalar flux per unit lethargy. (The 47-g structure is provided on Table 5.5.)
 - Deterministic codes: Multi-group normalized scalar flux per unit lethargy with their own group structure.
- Reaction rates
 - For the problems: **1C** and **1H**
 - For the burnup points: 1, 8, 13, 18, 23, 27, 31 and 35
 - 1-group absorption and fission reaction rates for each depletion zone
 - For nuclides: Table 5.6 provides the list of nuclides

5.4 Sensitivities

Sensitivity calculations need to be performed for the following parameters.

- Xenon
 - For the problems: **1C** and **2C**
 - All burnup points
 - Equilibrium xenon option
- Xenon
 - For the problems: **1C** and **2C**

- All burnup points
- Equilibrium xenon option
- Burnup intervals
 - For the problems: **1C**
 - All burnup points
 - Very fine burnup points: up to participants
- Number of intra depletion zones for gadolinia rod
 - For the problems: **1H**
 - All burnup points
 - 10 intra depletion zones

Table 5.4 Xenon option and editing parameters

No	Problem	Description	Xenon		Special option	Edit				
			Transient	Equilibrium		k_{eff}	Pin power	PND	Reaction rate	Flux
1	1A	Pin 3.1w/o $T_F=565K$	O			O				
2	1B	Pin 3.1w/o $T_F=600K$	O			O				
3	1C	Pin 3.1w/o $T_F=900K$	O	O	*A	O		O	O	O
4	1D	Pin 3.1w/o $T_F=1200K$	O			O				
5	1E	Pin IFBA 3.1w/o $T_F=565K$	O			O		O		
6	1F	Pin 3.6w/o $T_F=900K$	O			O				
7	1G	Pin 3.6w/o $T_F=900K$	O			O				
8	1H	Pin Gadolinia rod (5% Gd_2O_3)	O		*B	O		O	O	O
9	1I	Pin 3.1w/o $T_F=600/900/1200K$	O			O				
10	2A	FA No Poisons $T_F=565K$	O			O				
11	2B	FA No Poisons $T_F=600K$	O			O				
12	2C	FA No Poisons $T_F=900K$	O	O		O	O			
13	2D	FA No Poisons $T_F=1200K$	O			O				
14	2E	FA 12 Pyrex	O			O				
15	2F	FA 24 Pyrex	O			O	O			
16	2G	FA 24 AIC	O			O				
17	2H	FA 24 B4C	O			O				
18	2I	FA Instrument Thimble	O			O				
19	2J	FA Instrument + 24 Pyrex	O			O				
20	2K	FA Zoned + 24 Pyrex	O			O				
21	2L	FA 80 IFBA	O			O				
22	2M	FA 128 IFBA	O			O				
23	2N	FA 104 IFBA + 20 WABA	O			O	O			
24	2O	FA 12 Gadolinia	O			O				
25	2P	FA 24 Gadolinia	O			O	O			

*A: Burnup interval sensitivity calculation

*B: 10 intra pin subzones for gadolinia rod

Table 5.5 The 47-group boundaries

Gr	Upper (eV)								
1	2.00000E+07	11	2.03470E+03	21	5.71501E+00	31	1.07220E+00	41	1.45721E-01
2	6.06530E+06	12	1.30070E+02	22	5.04348E+00	32	1.01370E+00	42	1.11570E-01
3	3.67880E+06	13	7.88933E+01	23	4.45090E+00	33	9.71004E-01	43	8.19682E-02
4	2.23130E+06	14	4.78512E+01	24	3.92790E+00	34	9.09997E-01	44	5.69219E-02
5	1.35340E+06	15	2.90229E+01	25	2.38239E+00	35	7.82083E-01	45	4.27552E-02
6	8.20850E+05	16	1.37100E+01	26	1.85539E+00	36	6.25062E-01	46	3.06129E-02
7	4.97870E+05	17	1.20990E+01	27	1.45740E+00	37	5.03232E-01	47	1.23960E-02
8	1.83160E+05	18	8.31529E+00	28	1.23511E+00	38	3.57670E-01		1.00000E-05
9	6.73790E+04	19	7.33822E+00	29	1.16640E+00	39	2.70521E-01		
10	9.11880E+03	20	6.47602E+00	30	1.12540E+00	40	1.84430E-01		

Table 5.6 Nuclides for editing reaction rates

ID	Nuclide	ID	Nuclide	ID	Nuclide	ID	Nuclide
42095	⁹⁵ Mo	54135	¹³⁵ Xe	61148	¹⁴⁸ Pm	94238	²³⁸ Pu
43099	⁹⁹ Tc	55133	¹³³ Cs	62149	¹⁴⁹ Sm	94239	²³⁹ Pu
44101	¹⁰¹ Ru	55134	¹³³ Cs	63155	¹⁵⁵ Eu	94240	²⁴⁰ Pu
45103	¹⁰³ Rh	60143	¹⁴³ Nd	92235	²³⁵ U	94241	²⁴¹ Pu
46105	¹⁰⁵ Pd	60145	¹⁴⁵ Nd	92236	²³⁶ U	94242	²⁴² Pu
46107	¹⁰⁷ Pd	62150	¹⁵⁰ Sm	92238	²³⁸ U	95243	²⁴³ Am
46108	¹⁰⁸ Pd	62151	¹⁵⁰ Sm	93237	²³⁷ Np		

6. DISCUSSION

Currently the programs in Table 6.1 are supposed to be engaged in this code-to-code comparison for the depletion benchmark calculations.

Table 6.1 Transport depletion codes

Code	Solver			Developer	Group
	Transport	Depletion	Resonance		
MPACT	MOC	ORIGEN	Subgroup	CASL	47/51
SHIFT	Monte Carlo	ORIGEN		ORNL	CE
POLARIS	MOC	ORIGEN	ESSM	ORNL	252/56
TRITON	Monte Carlo	ORIGEN	CENTRM	ORNL	252/56
nTRACER	MOC	Krylov	Subgroup	SNU	47
McCARD	Monte Carlo	ORIGEN		SNU	CE
STREAM	MOC		Equivalence	UNIST	MG
SERPENT	Monte Carlo	CRAM		VTT	CE
MCNP6	Monte Carlo			LANL	CE

*ORIGEN: Exponential matrix + Bateman

ACKNOWLEDGEMENT

The author would like to acknowledge Kevin T. Clarno who is the CASL PHI lead for his efforts to review this document in detail and provide valuable comments.

REFERENCE

- [God14] Andrew T. Godfrey, "VERA Core Physics Benchmark Progression Problem Specifications," CASL-U-2012-0131-004, Rev. 4 (8/29/2014).
- [Wie14] W. Wieselquist, K. S. Kim , "Simplified Burnup Chain Development," CASL PHI Ticket#3432 (9/10/2014).

Appendix A. Constituent nuclides for the simplified burnup chain

No	Nuclide	CAT	ID	IFPY	Special Yield Definition ($ID_i/W_i/IFPY_i$)
1	5-B-0	1	50100	0	
2	5-B-10	1	50110	0	
3	8-O-16	1	80160	0	
4	47-Ag-107	1	471070	0	
5	47-Ag-109	1	471090	0	
6	47-Ag-110	1	471100	0	
7	48-Cd-110	1	481100	0	
8	48-Cd-111	1	481110	0	
9	48-Cd-112	1	481120	0	
10	48-Cd-113	1	481130	0	
11	48-Cd-114	1	481140	0	
12	48-Cd-115	1	481150	0	
13	49-In-113	1	491130	0	
14	49-In-115	1	491150	0	
15	62-Sm-152	1	621520	0	
16	62-Sm-153	1	621530	0	
17	63-Eu-151	1	631510	0	
18	63-Eu-152	1	631520	0	
19	63-Eu-152m	1	631521	0	
20	63-Eu-153	1	631530	0	
21	63-Eu-154	1	631540	0	
22	63-Eu-155	1	631550	0	
23	63-Eu-156	1	631560	0	
24	63-Eu-157	1	631570	0	
25	64-Gd-152	1	641520	0	
26	64-Gd-154	1	641540	0	
27	64-Gd-155	1	641550	0	
28	64-Gd-156	1	641560	0	
29	64-Gd-157	1	641570	0	
30	64-Gd-158	1	641580	0	
31	64-Gd-159	1	641590	0	
32	64-Gd-160	1	641600	0	
33	64-Gd-161	1	641610	0	
34	65-Tb-159	1	651590	0	
35	65-Tb-160	1	651600	0	
36	65-Tb-161	1	651610	0	
37	66-Dy-160	1	661600	0	
38	66-Dy-161	1	661610	0	
39	66-Dy-162	1	661620	0	
40	66-Dy-163	1	661630	0	
41	66-Dy-164	1	661640	0	
42	66-Dy-165	1	661650	0	
43	67-Ho-165	1	671650	0	
44	68-Er-162	1	681620	0	
45	68-Er-164	1	681640	0	
46	68-Er-166	1	681660	0	
47	68-Er-167	1	681670	0	
48	68-Er-168	1	681680	0	
49	68-Er-169	1	681690	0	
50	68-Er-170	1	681700	0	

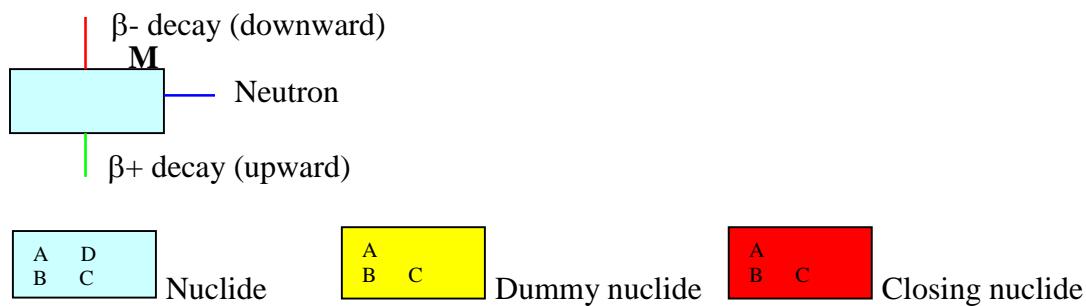
51	68-Er-171	1	681710	0
52	69-Tm-169	1	691690	0
53	69-Tm-170	1	691700	0
54	69-Tm-171	1	691710	0
55	72-Hf-174	1	721740	0
56	72-Hf-176	1	721760	0
57	72-Hf-177	1	721770	0
58	72-Hf-178	1	721780	0
59	72-Hf-179	1	721790	0
60	72-Hf-180	1	721800	0
61	72-Hf-181	1	721810	0
62	73-Ta-181	1	731810	0
63	73-Ta-182	1	731820	0
64	90-Th-230	2	902300	0
65	90-Th-231	2	902310	0
66	90-Th-232	2	902320	0
67	90-Th-233	2	902330	0
68	90-Th-234	2	902340	0
69	91-Pa-231	2	912310	0
70	91-Pa-232	2	912320	0
71	91-Pa-233	2	912330	0
72	91-Pa-234	2	912340	0
73	92-U-232	2	922320	0
74	92-U-233	2	922330	0
75	92-U-234	2	922340	0
76	92-U-235	2	922350	0
77	92-U-236	2	922360	0
78	92-U-237	2	922370	0
79	92-U-238	2	922380	0
80	92-U-239	2	922390	0
81	93-Np-236	2	932360	0
82	93-Np-237	2	932370	0
83	93-Np-238	2	932380	0
84	93-Np-239	2	932390	0
85	93-Np-240	2	932400	0
86	93-Np-240m	2	932401	0
87	94-Pu-236	2	942360	0
88	94-Pu-237	2	942370	0
89	94-Pu-238	2	942380	0
90	94-Pu-239	2	942390	0
91	94-Pu-240	2	942400	0
92	94-Pu-241	2	942410	0
93	94-Pu-242	2	942420	0
94	94-Pu-243	2	942430	0
95	95-Am-241	2	952410	0
96	95-Am-242	2	952420	0
97	95-Am-42m	2	952421	0
98	95-Am-243	2	952430	0
99	95-Am-244	2	952440	0
100	95-Am-44m	2	952441	0
101	96-Cm-242	2	962420	0
102	96-Cm-243	2	962430	0
103	96-Cm-244	2	962440	0

104	96-Cm-245	2	962450	0	
105	96-Cm-246	2	962460	0	
106	35-BR-81	3	350810	2	
107	35-BR-82	3	350820	2	
108	36-KR-82	3	360820	3	350821/0.024/1, 360820/1.000/1
109	36-KR-83	3	360830	2	
110	36-KR-84	3	360840	2	
111	36-KR-85	3	360850	2	
112	36-KR-86	3	360860	2	
113	38-SR-89	3	380890	2	
114	38-SR-90	3	380900	2	
115	39-Y-89	3	390890	1	
116	39-Y-90	3	390900	1	
117	39-Y-91	3	390910	2	
118	40-ZR-91	3	400910	1	
119	40-ZR-93	3	400930	2	
120	40-ZR-95	3	400950	2	
121	40-ZR-96	3	400960	2	
122	41-NB-95	3	410950	3	410950/1.000/1, 410951/0.944/1
123	42-MO-95	3	420950	3	410951/0.056/1, 420950/1.000/1
124	42-MO-96	3	420960	3	410960/1.000/1, 420960/1.000/1
125	42-MO-97	3	420970	2	
126	42-MO-98	3	420980	2	
127	42-MO-99	3	420990	2	
128	42-MO-100	3	421000	2	
129	43-TC-99	3	430990	1	
130	43-TC-99m	3	430991	1	
131	43-TC-100	3	431000	1	
132	44-RU-100	3	441000	1	
133	44-RU-101	3	441010	2	
134	44-RU-102	3	441020	2	
135	44-RU-103	3	441030	2	
136	44-RU-104	3	441040	2	
137	44-RU-105	3	441050	2	
138	44-RU-106	3	441060	2	
139	45-RH-102	3	451020	1	
140	45-RH-102m	3	451021	1	
141	45-RH-103	3	451030	1	
142	45-RH-103m	3	451031	1	
143	45-RH-104	3	451040	1	
144	45-RH-105	3	451050	1	
145	45-RH-105m	3	451051	1	
146	45-RH-106	3	451060	1	
147	45-RH-106m	3	451061	1	
148	46-PD-104	3	461040	1	
149	46-PD-105	3	461050	1	
150	46-PD-106	3	461060	1	
151	46-PD-107	3	461070	2	
152	46-PD-108	3	461080	2	
153	46-PD-109	3	461090	2	
154	47-AG-109	3	471090	1	
155	47-AG-109m	3	471091	1	
156	47-AG-110	3	471100	2	

157	47-AG-110m	3	471101	2	
158	47-AG-111	3	471110	2	
159	48-CD-110	3	481100	1	
160	48-CD-111	3	481110	3	471110/-1.000/2, 481110/1.000/2, 481111/1.000/1
161	48-CD-113	3	481130	2	
162	49-IN-115	3	491150	2	
163	51-SB-121	3	511210	2	
164	51-SB-123	3	511230	2	
165	51-SB-125	3	511250	2	
166	51-SB-127	3	511270	2	
167	52-TE-127	3	521270	-1	
168	52-TE-127m	3	521271	-1	
169	52-TE-129m	3	521291	2	
170	52-TE-132	3	521320	2	
171	53-I-127	3	531270	1	
172	53-I-128	3	531280	3	531280/0.931/2
173	53-I-129	3	531290	3	531290/1.000/2, 521291/-1.000/2
174	53-I-130	3	531300	2	
175	53-I-131	3	531310	2	
176	53-I-132	3	531320	1	
177	53-I-135	3	531350	2	
178	54-XE-128	3	541280	1	
179	54-XE-130	3	541300	1	
180	54-XE-131	3	541310	1	
181	54-XE-132	3	541320	1	
182	54-XE-133	3	541330	2	
183	54-XE-134	3	541340	2	
184	54-XE-135	3	541350	1	
185	54-XE-135m	3	541351	1	
186	54-XE-136	3	541360	2	
187	54-XE-137	3	541370	2	
188	55-CS-133	3	551330	1	
189	55-CS-134	3	551340	1	
190	55-CS-135	3	551350	1	
191	55-CS-136	3	551360	1	
192	55-CS-137	3	551370	1	
193	56-BA-134	3	561340	1	
194	56-BA-137	3	561370	1	
195	56-BA-140	3	561400	2	
196	57-LA-139	3	571390	2	
197	57-LA-140	3	571400	1	
198	58-CE-140	3	581400	1	
199	58-CE-141	3	581410	2	
200	58-CE-142	3	581420	2	
201	58-CE-143	3	581430	2	
202	58-CE-144	3	581440	2	
203	59-PR-141	3	591410	1	
204	59-PR-142	3	591420	1	
205	59-PR-143	3	591430	1	
206	59-PR-144	3	591440	1	
207	60-ND-142	3	601420	1	
208	60-ND-143	3	601430	1	
209	60-ND-144	3	601440	1	

210	60-ND-145	3	601450	2	
211	60-ND-146	3	601460	2	
212	60-ND-147	3	601470	2	
213	60-ND-148	3	601480	2	
214	60-ND-149	3	601490	2	
215	60-ND-150	3	601500	2	
216	60-ND-151	3	601510	2	
217	61-PM-147	3	611470	1	
218	61-PM-148	3	611480	-1	
219	61-PM-148m	3	611481	-1	
220	61-PM-149	3	611490	1	
221	61-PM-150	3	611500	1	
222	61-PM-151	3	611510	1	
223	62-SM-147	3	621470	1	
224	62-SM-148	3	621480	1	
225	62-SM-149	3	621490	1	
226	62-SM-150	3	621500	1	
227	62-SM-151	3	621510	1	
228	62-SM-152	3	621520	2	
229	62-SM-153	3	621530	2	
230	62-SM-154	3	621540	2	
231	62-SM-155	3	621550	2	
232	63-EU-151	3	631510	1	
233	63-EU-153	3	631530	1	
234	63-EU-154	3	631540	1	
235	63-EU-155	3	631550	1	
236	63-EU-156	3	631560	2	
237	63-EU-157	3	631570	2	
238	64-GD-154	3	641540	1	
239	64-GD-155	3	641550	1	
240	64-GD-156	3	641560	1	
241	64-GD-157	3	641570	1	
242	64-GD-158	3	641580	2	
243	64-GD-159	3	641590	2	
244	64-GD-160	3	641600	2	
245	64-GD-161	3	641610	2	
246	65-TB-159	3	651590	1	
247	65-TB-160	3	651600	1	
248	65-TB-161	3	651610	1	
249	66-DY-160	3	661600	1	
250	66-DY-161	3	661610	1	
251	66-DY-162	3	661620	2	
252	66-DY-163	3	661630	2	
253	66-DY-164	3	661640	2	
254	66-DY-165	3	661650	2	
255	67-HO-165	3	671650	3	661651/0.022/2, 671650/1.000 /1

Appendix B. Depletion chain



A : Nuclide

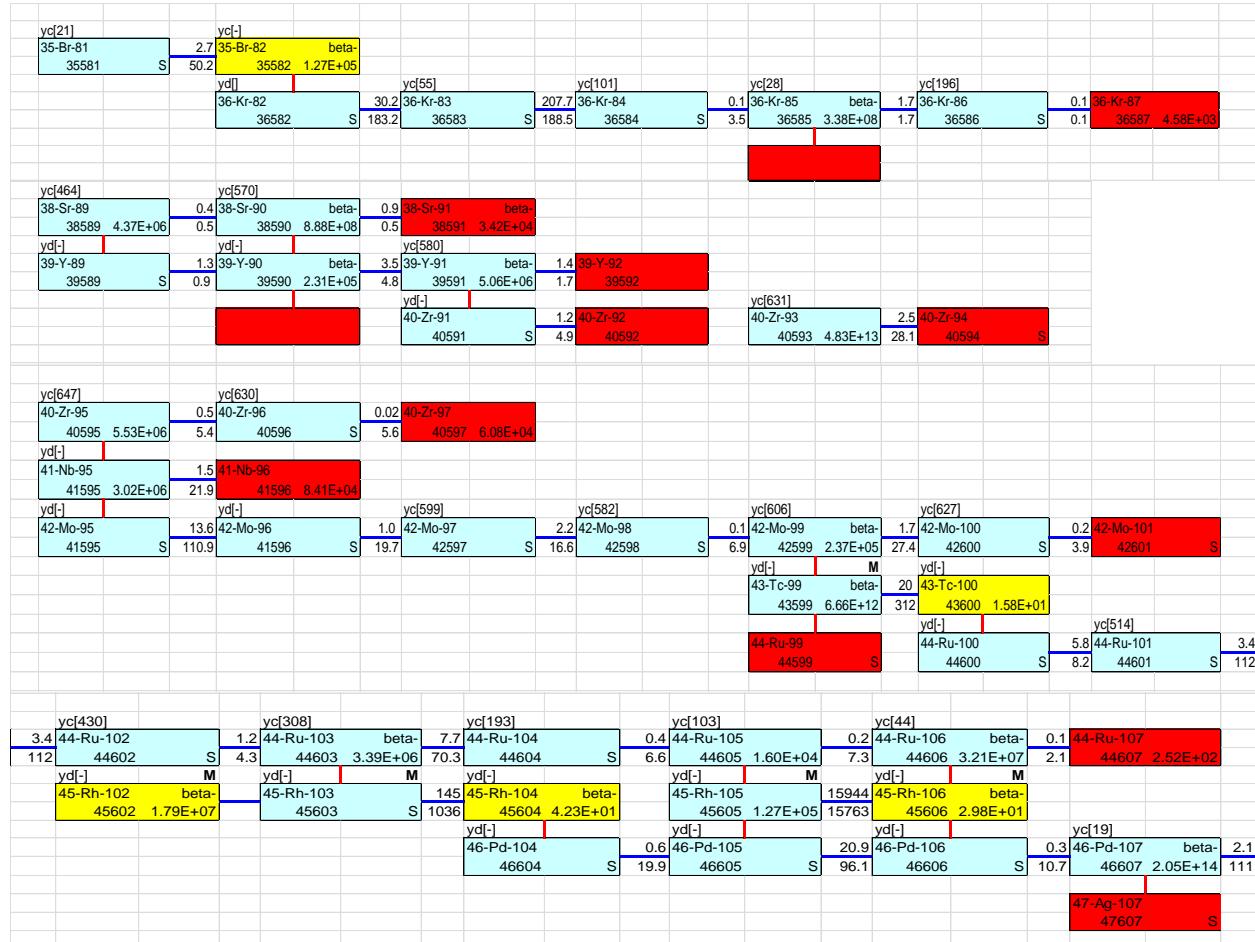
B : Nuclide Id. in library

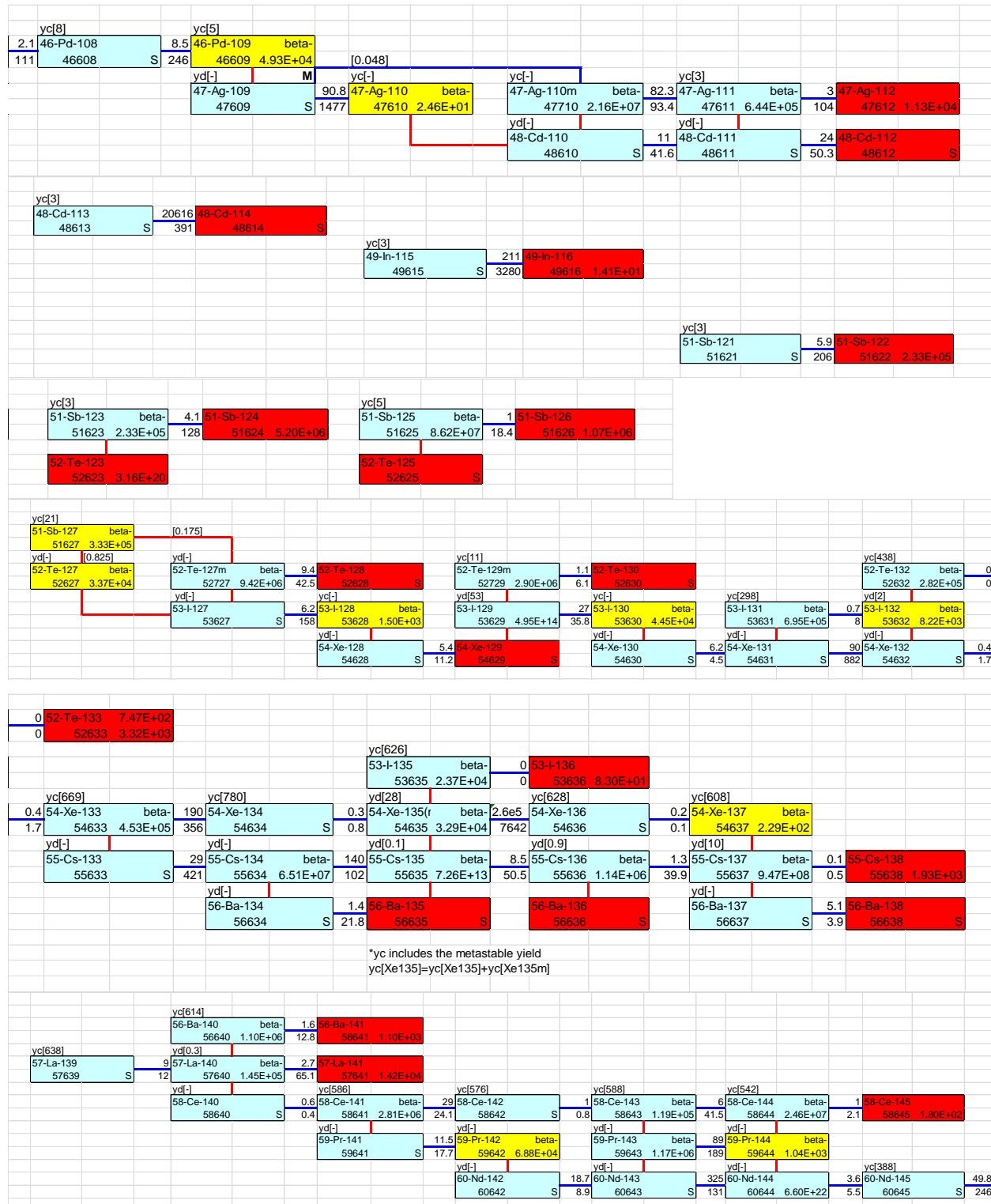
C : Decay half life (s)

D : Decay type

M : Both stable and meta-stable

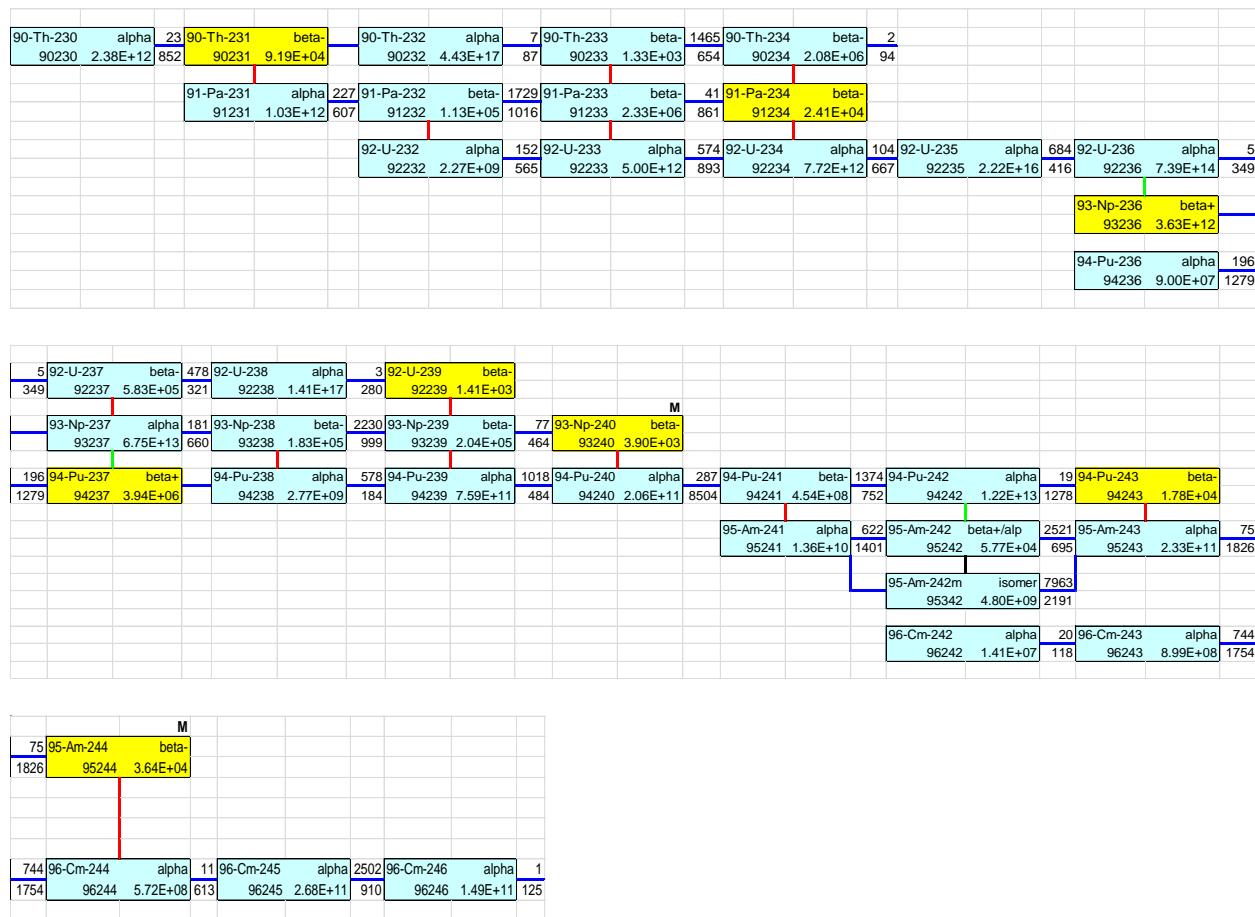
[Depletion chain of fission product nuclides]





yc[297]	yd[222]							
49.8 60-Nd-146 246 60646 S	1.4 60-Nd-147 3.1 60647 9.49E+05	440	574					
yd[-] 61-Pm-147 61647 8.28E+07	168 2124							
yd[-] 62-Sm-147 62647 3.35E+18	50 779							
yc[222]	yc[167]	yc[107]	yc[66]	yc[42]				
60-Nd-147 60647 9.49E+05	440 574	2.5 60-Nd-149 60648 6.21E+03	1.2 60-Nd-150 60650 7.46E+02	16 60-Nd-151 60651 1.02E+05	700 61-Pm-152 61651 2.46E+02			
yd[-] 61-Pm-147 61647 8.28E+07	0.472 61-Pm-148m 61748 3.57E+06	0.046 61-Pm-148 61648 4.64E+05	2000 61-Pm-149 61649 1.91E+05	1400 61-Pm-150 61650 9.65E+03	801 61-Pm-151 61651 2.84E+09	2004 61652 2.46E+02		
yd[-] 62-Sm-147 62647 3.35E+18	0.528 0.954	2.7 62-Sm-149 62648 2.50E+23	27.7 62-Sm-150 3463 6.31E+22	40148 62-Sm-150 3463 62650 S	100 62-Sm-151 62651 3.34E+09	15204 62-Sm-152 3433 62652 S	206 63-Eu-151 63651 S	2977 63-Eu-152 4.29E+08 63652 3.36E+04
yc[16]	yc[7]	yc[3]	yc[2]	yc[0.7]	yc[0.4]	yc[0.1]	yc[0.1]	
206 62-Sm-153 2977 62653 1.67E+05	330 62-Sm-154 2862 62654 S	5.5 62-Sm-155 33.9 62655 1.34E+03	3756 63-Eu-156 1360 63655 1.48E+08	482 63-Eu-157 15319 63656 1.31E+06	190 63-Eu-158 1492 63657 5.46E+04	1302 63658 2.75E+03	2 64-Gd-159 63 64659 6.68E+04	
yd[-] 63-Eu-153 63653	312 63-Eu-154 1429 63654 2.71E+08	1840 63-Eu-155 1360 63655 1.48E+08	60896 64-Gd-156 1543 64655 S	1.7 64-Gd-157 105 64657 S	2.564 64-Gd-158 755 64658 S	yd	65-Tb-159 65659 S	26 460
yc[0.1]	yc[-]							
64-Gd-160 64660 S	0.8 64-Gd-161 7.9 64661 2.19E+02							
yd[-] 65-Tb-160 460 65660 6.25E+06	525 65-Tb-161 1135 65661 5.96E+05	65-Tb-162 65662 4.48E+02						
yd[-] 66-Dy-160 66660 S	57 66-Dy-161 1108 66661 S	600 66-Dy-162 1087 66662 S	194 66-Dy-163 2746 66663 S	124 66-Dy-164 1489 66664 S	2651 66-Dy-165 342 66665 8.40E+03			
yd[-] 67-Ho-165 67665 S					63.4 67-Ho-166 9.65E+04 675 67166 3.79E+10			

[Depletion chain of heavy metal nuclides]



[Depletion chain of activation nuclides]

