

CREATION OF THE EQUILIBRIUM CORE PBMR ORIGEN-S CROSS SECTION LIBRARY

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ABSTRACT

As part of the design calculations for the Pebble Bed Modular Reactor (PBMR), fuel inventories, neutron and gamma sources and decay heat needs to be determined for the fuel spheres. Using the SCALE4.4 code system, a PBMR specific cross section library was created for the ORIGEN-S depletion calculations, assuming a 10-pass refueling system for the PBMR. In this paper the rationale for the creation of the PBMR library is evaluated in terms of the spectrum dependence due to burn-up. The ORIGEN-S PBMR library was further evaluated comparing the results for different parameters calculated with the reactor analysis diffusion code VSOP and the Monte Carlo code MCNP4C.

1. Introduction

The Pebble Bed Modular Reactor (PBMR) design applies a continuous reloading scheme where unloaded fuel spheres, which have not reached the target burn-up, are returned to the top of the core. For a so-called 10-pass equilibrium core this implies that the fuel spheres will circulate ten times, on average, through the core. In practice it means that fuel spheres at different burn-up surround any single fuel sphere. As part of the PBMR design calculations the fuel sphere inventories, neutron and gamma sources and decay heat needs to be determined as a function of burn-up. In order to solve the burn-up equations, spectrum averaged neutron interaction cross sections are required. However, due to the changes in the isotope concentrations with burn-up, the neutron spectrum, and thus the spectrum averaged cross sections, becomes burn-up dependent. Therefore, when creating a cross section library, the spectrum dependence due to burn-up needs to be determined.

The depletion and decay calculations for the PBMR design are performed using the ORIGEN-S module of the SCALE4.4 [1] code system. The reliability of the ORIGEN-S results depends mainly on the appropriateness of the neutron cross section library used for the calculations.

In Section 2 the rationale for the creation of the PBMR library is evaluated in terms of the spectrum dependence due to burn-up. Based on these conclusions a PBMR specific ORIGEN-S library has been created for a 1 dimensional PBMR model described in Section 3. The PBMR library was evaluated comparing the one energy group ORIGEN-S neutron interaction cross sections with the cross sections obtained from the reactor analysis diffusion code VSOP [2,3] and the Monte Carlo code MCNP4C [4,5]. In Section 4 comparisons are provided for the ORIGEN-S and VSOP depletion calculations. Section 5 contains the conclusions.

2. PBMR Library Generation Rationale

Within the traditional PWR fuel assembly reload methodology the ORIGEN-S cross section libraries are often created with the assumption that the neutron spectrum within the fuel assembly is dominated by the burn-up of the fuel assembly itself and that the specific burn-up of the surrounding assemblies are less important. However, with the small PBMR fuel spheres (assemblies) and the graphite moderation environment, the PWR approach might not be valid. While evaluating the PBMR 10-pass continuous reloading scheme, it became evident that the flux spectrum within a fuel sphere was mostly

determined by the burn-up of the surrounding spheres, while the burn-up of the fuel sphere itself only had a secondary effect on the spectrum.

In the 10-pass PBMR continuous reloading scheme a fuel sphere will on average reach its target burn-up (80 GWD/TU) after ten circulations. The average burn-up for the upper layer of fuel spheres is about 41 GWD/TU, ranging from zero up to about 74 GWD/TU burn-up. The average burn-up of the bottom fuel layer is about 49 GWD/TU. Thus, a fuel sphere burning over its life from zero up to 80 GWD/TU will always be surrounded by fuel spheres being at an average burn-up between 41 GWD/TU and 49 GWD/TU.

For the evaluation of the cross section spectrum dependence due to burn-up, a spherical reactor model was constructed consisting of a single fuel sphere in the center, surrounded by a 1 m fuel driver zone and a 1 m graphite reflector. Using the flux spectrum within the central fuel sphere, ORIGEN-S cross section libraries has been generated for the following cases:

- REF** The central fuel sphere and the driver fuel zone at equilibrium (45 GWD/TU) burn-up
- A-1** The central fuel sphere at 0 GWD/TU surrounded by fuel spheres at 45 GWD/TU burn-up
- A-2** The central fuel sphere at 80 GWD/TU surrounded by fuel spheres at 45 GWD/TU burn-up
- B-1** The central fuel sphere at 45 GWD/TU surrounded by fuel spheres at 0 GWD/TU burn-up
- B-2** The central fuel sphere at 45 GWD/TU surrounded by fuel spheres at 80 GWD/TU burn-up

All the SCALE calculations were performed in 238 energy groups using the 238-GROUP ENDF/B-V library from the SCALE system. All the isotopes treated explicitly in the VSOP calculation, and available in the SCALE 238-Group library, were specified. Additional fission product isotopes (with negligibly small atom densities) were also specified for the central fuel sphere to enable an update of the ORIGEN-S cross sections for these isotopes. These fission product isotopes were specified due to its importance with regard to the burn-up measurements. Using the 238 energy group flux spectrum, calculated for the central fuel sphere in the spherical reactor model, the isotopic cross sections were collapsed to the ORIGEN-S 3 energy group structure. The ORIGEN-S cross section library was then updated by replacing the original ORIGEN-S cross sections with the 3 group cross sections for all the isotopes specified in the single fuel sphere. The ORIGEN-S cross sections (the updated and not updated) were then collapsed to one energy group using the 3 group spectrum in the single fuel sphere.

Using the different ORIGEN-S libraries created for the central fuel sphere, the burn-up was performed for 874 days, irradiating at a thermal flux (<0.5 eV) of $6.3 \times 10^{13} \text{ n.cm}^{-2}.\text{s}^{-1}$. However, for these relative comparisons the exact flux used for the ORIGEN-S burn-up calculation is not important. The activities and masses obtained for the reference ORIGEN-S library are tabulated in Table 1 for a selection of isotopes. The percentage differences with respect to the reference case (REF) are provided for the different ORIGEN-S libraries.

The percentage differences in Table 1 clearly shows that the results for cases A-1 and A-2 are much closer to the REF case than cases B-1 and B-2. Also, when burning cases B-1 and B-2 to the REF target burn-up, the differences have decreased but were still large in comparison with cases A-1 and A-2. Thus, it can be concluded that the burn-up of the surrounding spheres on the spectrum within the specific sphere is much more important than the burn-up of the sphere itself.

The reason for the spectrum within a fuel sphere to be mainly dependent on the burn-up of the surrounding fuel spheres is due to the large scattering to absorption ratio in graphite and that the UO_2 micro-kernels are relatively far apart (packing ratio 0.015). The scattering mean free path for thermal neutrons in carbon is about 2.6 cm, while the absorption mean free path is about 31 m. This implies that neutrons originating from fuel spheres relatively far from a specific fuel sphere, can also contribute to the spectrum within the fuel sphere.

Table 1 ORIGEN-S results for 874 days burn-up (thermal flux $6.3 \times 10^{13} \text{ n.cm}^{-2}.\text{s}^{-1}$)

Library Case	A-1	A-2	REF	B-1	B-2
Central Fuel Burn-up (GWD/TU)	0	80	45	45	45
Driver Fuel Burn-up (GWD/TU)	45	45	45	0	80
Activities	%	%	Bq	%	%
Sr-90	0.0	0.0	6.4×10^{10}	1.2	-1.8
Nb-97	0.0	-0.4	9.8×10^{11}	3.4	-6.8
Ag-110m	1.2	-1.3	2.5×10^9	11	-21
I-131	0.0	0.0	6.2×10^{11}	3.6	-7.7
I-132	0.0	0.0	9.1×10^{11}	4.1	-7.4
I-133	0.0	-0.3	1.3×10^{12}	3.5	-7.3
Cs-134	1.8	-1.8	1.1×10^{11}	6.3	-12
Cs-137	0.0	0.0	8.8×10^{10}	2.5	-4.4
Ba-137m	0.0	0.0	8.3×10^{10}	2.7	-4.7
Ce-143	0.0	-0.4	9.4×10^{11}	3.2	-6.3
TOTAL	0.3	0.0	1.1×10^{14}	3.8	-6.6
Mass	%	%	gram	%	%
U-235	0.6	-0.6	0.158	-0.6	1.3
U-238	0.1	0.1	7.82	-0.3	0.6
Pu-239	-1.0	0.0	0.0502	4.4	-10
Pu-241	0.4	-0.4	0.0246	6.9	-13
Heavy metal	0.0	0.0	8.22	-0.1	0.4
Burn-up	%	%	GWD/TU	%	%
	0.04	-0.1	80.06	2.5	-4.6

Similarly, ORIGEN-S cross section libraries have been created for the central fuel sphere (equilibrium burn-up) surrounded, respectively, by spheres at 41 GWD/TU (average upper layer burn-up) and spheres at 49 GWD/TU (average bottom layer burn-up). The ORIGEN-S activities and masses calculated for these two libraries compares within 1 %.

In conclusion, the use of a single ORIGEN-S cross section library, generated for the 10-pass PBMR design at equilibrium burn-up conditions, should be acceptable for most practical applications.

3. PBMR ORIGEN-S Library

Based on the conclusion in Section 2, an equilibrium core PBMR ORIGEN-S cross section library has been created with a 1-dimensional cylindrical PBMR reactor model. Table 2 provides a summary of the model. All fuel spheres were at equilibrium core burn-up (~45 GWD/TU) with the isotopic atom densities provided in Reference [3].

Table 2 PBMR cylindrical model used in SCALE

Region	Radius (cm)	Material
Central column	87.5	100% graphite spheres
Mixed region	112.5	50% graphite & 50% fuel spheres
Fuel region	175.0	100% fuel spheres
Reflector	275.0	Graphite (1.7 g.cm^{-3})

In reference [6] it is stated that the SCALE Dancoff factor calculation for tiny fuel kernels dispersed in graphite with a large number of equivalent unit cells per mean free path is questionable. The Dancoff factors derived from reference [6] for the PBMR fuel compares well with the VSOP Dancoff factors. A summary of the Dancoff factors are tabulated in Table 3.

Table 3 Dancoff factors for fuel spheres

Origin	Infinite system of microspheres	Infinite system of fuel spheres
SCALE	0.882	same as microspheres
VSOP	0.512	0.405
Reference [6]	~ 0.52	~ 0.42

A PBMR ORIGEN-S library has been created for both the SCALE and VSOP Dancoff factors, called D_{SCALE} and D_{VSOP} . In Table 4 the ORIGEN-S fuel zone microscopic cross sections are tabulated together with the VSOP and MCNP calculated values. The VSOP and MCNP values were obtained for 3-dimensional PBMR models.

Table 4 Microscopic fuel zone cross sections calculated with SCALE, MCNP and VSOP

REACTION	SCALE (D_{SCALE})	SCALE (D_{VSOP})	MCNP*	VSOP
	1173K	1173K	1200K	~1100K
U-235 (n,g) U-236	22.7	22.3	20.9	22.3
U-235 (n,fission)	109.0	106.8	105.2	105.5
U-238 (n,g) U-239	2.63	3.47	3.45	3.45
U-238 (n,fission)	2.46e-2	2.54e-2	2.73e-2	2.35e-2
Pu-239 (n,g) Pu-240	267.8	262.1	262.9	264.2
Pu-239 (n,fission)	432.9	423.7	428.7	425.3
Pu-241 (n,g) Pu-242	145.6	142.6	128.3	126.8
Pu-241 (n,fission)	370.0	362.3	355.5	358.5

* Nominal relative error of 0.2%

Comparing the SCALE (D_{VSOP}), MCNP and VSOP cross sections for the fuel zone, the values are of the same order. The SCALE (D_{VSOP}) and VSOP values compare well, except for the Pu-241 capture cross section, which differs with 12%. Further evaluation for this difference falls outside the scope of this paper.

The SCALE cross sections calculated, respectively, for D_{SCALE} and D_{VSOP} compare reasonably well, except for the U-238 capture cross section that differs with 32%. This is as expected since the U-238 resonance shielding is dominant for low enriched uranium fuel. This is also the reason why resonance shielding in VSOP is only taken into account for the U-238 capture cross section.

Similarly the SCALE, VSOP and MCNP cross sections have been compared for the mixed fuel region. The cross section differences were of the same order as for the fuel region.

From the comparisons above, the neutron interaction cross sections in the PBMR ORIGEN-S library seems to compare favorably with VSOP and MCNP. In Section 4 the PBMR ORIGEN-S library, created with SCALE using the D_{VSOP} value, is evaluated for burn-up calculations.

4. ORIGEN-S Burn-up Comparisons with VSOP

The PBMR ORIGEN-S library, created with D_{VSOP} , was evaluated by comparing different ORIGEN-S burn-up results with VSOP. Parameters compared are burn-up and actinide masses. To determine the thermal flux below 0.5 eV, which is used as ORIGEN-S input, the flux spectra calculated with MCNP, SCALE (D_{VSOP}) and VSOP were at first compared for the VSOP energy group structure. These results are tabulated in Table 5.

Table 5 Fuel region flux spectra for the VSOP energy group structure

Energy	VSOP	SCALE (D_{VSOP})	MCNP*
10 MeV - 0.1 MeV	0.167	0.176	0.183
0.1 MeV - 29 eV	0.287	0.278	0.288
29 eV - 1.86 eV	0.070	0.070	0.072
1.86 eV - 0 eV	0.476	0.476	0.457

* Nominal relative error of 0.2%

The results in Table 5 show that the flux spectra calculated with VSOP, SCALE (D_{VSOP}) and MCNP compares reasonably well, specially the thermal flux fraction (<1.86 eV) for VSOP and SCALE. Based on this it should be reasonable to assume that the SCALE thermal flux fraction below 0.5 eV (namely 0.42) can be used for the ORIGEN-S burn-up calculations. Therefore, the ORIGEN-S depletion calculations have been performed specifying the ORIGEN-S thermal flux as 42% of the VSOP fuel region axially dependent total flux values.

The end-of-pass burn-up values calculated with ORIGEN-S and VSOP for the 10 passes, are tabulated in Table 6. In Table 7 the end-of-life masses calculated with VSOP and ORIGEN-S are tabulated for U-235, U-238, Pu-239 and Pu-241.

Table 6 End-of-pass fuel sphere burn-up (GWD/TU) calculated with ORIGEN-S and VSOP

Pass	ORIGEN-S	VSOP	Pass	ORIGEN-S	VSOP
1	10.7	10.9	6	54.8	55.0
2	21.0	21.2	7	61.8	62.0
3	30.5	30.7	8	68.2	68.4
4	39.3	39.5	9	74.3	74.4
5	47.3	47.6	10	80.0	80.1

Table 7 ORIGEN-S and VSOP actinide masses (g) after 874 days burn-up

Isotope	ORIGEN-S	VSOP	% Difference
U-235	0.133	0.119	11.8
U-238	7.90	7.92	-0.3
Pu-239	0.0413	0.0374	10.4
Pu-241	0.0195	0.0199	-2.0
Total	8.25	8.15	1.2 %

The burn-up values as tabulated for ORIGEN-S and VSOP in Table 6 correspond well. The actual mass differences (Table 7) between the ORIGEN-S and VSOP values are up to 10 %. However, since the actual fission product yields for the different fissionable isotopes generally do not differ too much, it can be expected that the ORIGEN-S and VSOP fission products should compare well within 10%.

5. Conclusions

In this paper the creation of the PBMR library was evaluated in terms of the spectrum dependence due to burn-up. The results clearly showed that the flux spectrum within a fuel sphere is dominated by the average spectrum of all fuel spheres around the sphere. In most cases the resulting error for not taking the spheres own burn-up into account in the spectrum calculation will be less than 1%.

Following on this, a single equilibrium PBMR ORIGEN-S cross section library has been created for a 1-dimensional cylindrical model, based on the VSOP PBMR model. The ORIGEN-S PBMR library was evaluated comparing cross sections, fluxes, fission product activities, actinide masses and burn-up with results obtained from VSOP and MCNP-4C.

Based on the results obtained, the equilibrium core PBMR ORIGEN-S cross section library can be used with confidence for the 10-pass PBMR fuel depletion calculations.

6. Acknowledgement

The authors would like to thank PBMR Pty Ltd for their financial support and permission to publish this work.

7. References

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