Preliminary Neutronics Design and Analysis of D₂O Cooled High Conversion PWRs

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SUMMARY

This report presents a neutronics analysis of tight-pitch D₂O-cooled PWRs loaded with MOX fuel and focuses essentially on the Pu breeding potential of such reactors as well as on an important safety parameter, the void coefficient, which has to be negative. It is well known that fast reactors have a better neutron economy and are better suited than thermal reactors to breed fissile material from neutron capture in fertile material. Such fast reactors (e.g. sodium-cooled reactors) usually rely on technologies that are very different from those of existing water-cooled reactors and are probably more expensive.

This report investigates another possibility to obtain a fast neutron reactor while still relying mostly on a PWR technology by:

- (1) Tightening the lattice pitch to reduce the water-to-fuel volume ratio compared to that of a standard PWR. Water-to-fuel volume ratios of between 0.45 and 1 have been considered in this study while a value of about 2 is typical of standard PWRs,
- (2) Using D₂O instead of H₂O as a coolant. Indeed, because of its different neutron physics properties, the use of D₂O hardens the neutron spectrum to an extent impossible with H₂O when used in a tight-pitch lattice.

The neutron spectra thus obtained are not as fast as those in sodium-cooled reactor but they can still be characterized as fast compared to that of standard PWR neutron spectra.

In the phase space investigated in this study we did not find any configurations that would have, at the same time, a positive Pu mass balance (more Pu at the end than at the beginning of the irradiation) and a negative void coefficient. At this stage, the use of radial blankets has only been briefly addressed whereas the impact of axial blankets has been well defined.

For example, with a D₂O-to-fuel volume ratio of 0.45 and a core driver height of about 60 cm, the fissile Pu mass balance between the fresh fuel and the irradiated fuel (50 GWd/t) would be about -7.5% (i.e. there are 7.5% fewer fissile Pu isotopes at the end than at the beginning of the irradiation) and the void coefficient would be negative. The addition of 1 cm of U-238 blanket at the top and bottom of the fuel would bring the fissile Pu mass balance from -7.5% to -6.5% but would also impact the void coefficient in the wrong way. In fact, it turns out that the void coefficient is so sensitive to the presence of axial blanket that it limits its size to only a few cm for driver fuel height of about 50-60 cm. For reference, the fissile Pu mass balance is about -35% in a standard PWR MOX fuel such as those used in France.

In order to reduce the fissile Pu deficit and potentially reach a true breeding regime (i.e. a positive Pu mass balance), it would be necessary to make extensive use of radial blankets, both internal and external. Even though this was not addressed in detail here, it is reasonable to believe that at least as much U-238 blanket subassemblies as MOX driver fuel subassemblies would be necessary to breed enough Pu to compensate for the Pu deficit in the driver fuel. Hence, whereas a relatively simple D₂O-cooled PWR core design makes it possible to obtain a near-breeder core, it may be necessary to more than double the mass of heavy metal in the core as well as the mass of heavy metal to reprocess per unit of energy produced in order to breed the few percents of Pu missing to reach a true breeding regime. It may be interesting to quantify these aspects further in the future.

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FUEL CYCLE OPTIONS/FUEL CYCLE PERFORMANCE AND ANALYSIS

PRELIMINARY NEUTRONICS DESIGN AND ANALYSIS OF D₂O COOLED HIGH CONVERSION PWRs

1. INTRODUCTION

There has been growing interest in studying the feasibility of reduced-moderation PWRs and BWRs in order to establish the sustainable nuclear fuel-cycle using existing water-cooled reactor technology, which could be the potential alternative to fast reactor based fuel cycle options [1-10]. The design targets of such reactors are to obtain high Pu conversion ratio while retaining the negative void reactivity. In this work, we will perform preliminary analyses of D₂O cooled PWR in order to investigate fundamental neutronics characteristics of this type of reactors by particularly targeting on reactors having smaller sized cores (less than 10 m³). The vast majority of these studies considered only light water (H₂O) whereas there has been limited number of studies done for heavy water (D₂O) as a means to harden the neutron spectrum [2-4, 8, 9]. The reason could be because of its reputation of “best neutron moderator” as well as its higher cost compared to H₂O.

The “best neutron moderator” reputation is justified because of its very small neutron capture cross-section and because deuterium is one of the lightest elements, second only to hydrogen, hence allowing to reach criticality even with natural uranium (because of its high neutron capture cross-section hydrogen is not considered as good of a moderator). However, in order to take advantage of its good neutron moderation properties, it is necessary to have large volumes of D₂O because the elastic scattering cross-section of deuterium in the slowing-down energy range is only about 4 barns against about 20 barns for hydrogen. The difference in the neutron elastic scattering cross-sections of H₂O and D₂O is the reason for the different sizes of PWRs and CANDUs; for the same power CANDUs need to be larger than PWRs to allow enough space for the neutrons to slowdown to the thermal energy.

One of aspects necessary to achieve the design target of high-conversion reactors is the hardening of neutron spectrum in order to increase the conversion of U-238 into Pu-239. One can obtain the harder spectrum by either reducing the moderator-to-fuel volume ratio (i.e., tightening the fuel pin pitch) or using the moderators that are more transparent to neutron than H₂O. For instance, if H₂O is replaced by D₂O in a PWR or BWR lattice, the resulting neutron spectrum will be substantially harder. This is illustrated by Figure 1 showing the neutron spectra in PWR lattices characterized by water-to-fuel volume ratios of 2 (value corresponding to actual operating PWRs), 1 and 0.6. There are some visible thermal peaks that can be observed when the water-to-fuel volume ratio is 2 or 1 in H₂O whereas none of them can be seen in D₂O moderator. Thus, the use of D₂O hardens the neutron spectrum to an extent impossible with H₂O.

Figure 1. Neutron spectra with different moderator-to-fuel volume ratios.

Figure 2 shows the average unit cell spectra in different types of coolants. The sodium coolant gives the hardest spectrum in this figure. However, only the small difference can be observed between the sodium cooled case and voided core. This indicates that the void reactivity of sodium cooled core is always small and likely to be positive caused by slight increase of the neutron generation per absorption, η , in the voided core [8]. The spectra could be also hardened by the light water and heavy water moderators with tighter fuel pin pitch as shown in Figure 1; however, they are not as hard as the spectrum in the sodium cooling case. The large spectrum shift due to voiding of the core indicates that the reduced moderation water reactors could be still sensitive to core configurations and compositions like existing water reactors; however, they have potential to retain negative void reactivity.

Figure 2. Neutron spectra obtained by CENTRM [11] unit cell calculations with different coolant types (moderator-to-fuel volume ratio = 0.6).

This report presents the preliminary studies for the design of D₂O-cooled PWRs in U-Pu cycle aiming at high Pu conversion ratio and negative void reactivity. Some recent studies done by other groups have shown the conceptual designing of the same type of reactors using the large sized core [2, 3]. This work focuses on small sized cores (less than 10 m³) in order to ensure a negative void coefficient. The analyses in this preliminary work have been carried out using Monte Carlo based burnup calculations with sets of simplified computational models. Section 2 of this report contains a discussion of the optimum core configurations that have negative void coefficients. Section 3 documents the performance of axial, internal, and radial blankets by burnup calculations with 3D pin-cell models. Also the burnup calculations for the simple assembly models with seed and blanket fuel pins will be shown in Section 3. Finally, the conclusion will be provided in Section 4.

2. DETERMINATION OF OPTIMUM CORE CONFIGURATION

2.1 Methodology

A set of criticality calculations has been performed for selected core configurations in order to determine their void coefficients and necessary Pu content. We have selected SCALE6.1 code system [11] to perform all calculations because of its capability to handle complicated reactor physics and criticality safety analyses by several modules in user friendly manner. Calculations for the determination of void coefficients have been performed by Monte Carlo based criticality analysis module CSAS5 sequence as shown in Figure 3. In this scheme, the calculation is started from the unit cell self-shielding calculations. Then, the unit cell is homogenized by means of the solution of the unit cell calculations. After that, the resonance corrected 238-group library is used for the KENO-V.a. criticality calculations in cylindrical geometry. While this procedure ignores some details such as fuel assembly calculations, it will provide us roughly estimated core neutronic characteristics and is sufficient for this preliminary study.

Figure 3. Calculation sequence for determining void coefficients by SCALE6 (CSAS5).

The enrichment of the fuel has been determined for each core to be able to obtain k_{eff} of 1.02 based on an initial guess of reactivity swing per cycle. As will be shown later on, this value is somewhat too low and, consequently, the Pu contents calculated are also too low. Nevertheless, the trends shown in this chapter are useful to understand the physics. The fuel (Pu and depleted U) compositions are shown in Table 1. A set of criticality calculations for voided cores has been performed by multiplying the nominal D₂O density of the reference core by voiding factors (namely 0.7, 0.1, 0.075, 0.05, and 0.02). Then, we define the void coefficient as:

$$C_v = \frac{k_{\text{eff}}^{\text{voided}} - k_{\text{eff}}^{\text{reference}}}{k_{\text{eff}}^{\text{voided}} k_{\text{eff}}^{\text{reference}}} \times 10^5 \quad [\text{pcm}] \quad (1)$$

Since in Eq. (1), each k_{eff} has a statistical error from KENO-V.a. Monte Carlo calculation, the void coefficient also contains the statistical error. Therefore, the statistical error of the void coefficients can be obtained by the error propagation:

$$\sigma_{C_v} = 10^5 \sqrt{\frac{\sigma_{k_{\text{eff}}^{\text{voided}}}^2}{k_{\text{eff}}^{\text{voided}^4}} + \frac{\sigma_{k_{\text{eff}}^{\text{reference}}}^2}{k_{\text{eff}}^{\text{reference}^4}}} \quad (2)$$

Table 1. Isotopic composition of the MOX fuel.

Isotopes	Pu [wt% of Pu]	Depleted U [wt% of U]
²³⁸ Pu	2.6	—
²³⁹ Pu	54.3	—
²⁴⁰ Pu	25.9	—
²⁴¹ Pu	8.7	—
²⁴² Pu	7.62	—
²⁴¹ Am	0.88	—
²³⁵ U	—	0.25
²³⁸ U	—	99.75

2.2 Core without Axial Blanket

We have started from the determination of the optimum base core configurations that give the sufficiently large negative void reactivity at the beginning of the core life (BOL). A simple cylindrical base core configuration as shown in Figure 4 has been considered. Each core is surrounded by 20cm-thick D₂O shield both radially and axially. In all core configurations, unit pin-cells are considered to be arranged in the triangular pitched array, which can effectively reduce the water-to-fuel volume ratio. We have considered water-to-fuel volume ratios of 0.45, 0.6 and 1.0 while the fuel pin diameter and stainless steel (SS) clad thickness are kept as 0.836 cm and 0.057cm, respectively. The temperature of U-Pu fuel is set to 1123.15 °K, and that of other regions (SS clad, D₂O coolant and shield) is set to 580.15 °K. Table 2 shows the initially selected list of core dimensions without blanket.

Figure 4. Cylindrical base core configuration.

Table 2. Initial selection of core dimensions without blanket.

Core Number	Volume [m ³]	H/D	H [cm]	D [cm]	W/F
1	10	0.25	92.67	370.67	0.6
2	10	0.25	92.67	370.67	1
3	10	0.225	86.382	383.922	0.6
4	10	0.225	86.382	383.922	1
5	10	0.2	79.858	399.294	0.6
6	10	0.2	79.858	399.294	1
7	7.5	0.25	84.194	336.778	0.6
8	7.5	0.25	84.194	336.778	1
9	7.5	0.225	78.484	348.816	0.6
10	7.5	0.225	78.484	348.816	1
11	7.5	0.2	72.556	362.784	0.6
12	7.5	0.2	72.556	362.784	1
13	7.5	0.2	72.556	362.784	0.45
14	7.5	0.175	66.376	379.296	0.45
15	7.5	0.15	59.894	399.294	0.45
16	5	0.2	63.384	316.92	0.6

Table 3 shows void coefficients for 10 m³ cores (cores 1-6) calculated by KENO-V.a. For the verification and quick comparison, we have also performed deterministic calculations using ERANOS2.2 [12], which is well-known for the analysis of fast reactor core designs. The ERANOS calculation consists of 1968-group ECCO unit-cell self-shielding calculation, which collapses the number of energy groups down to 33 groups, and BISTRO S_{16} RZ deterministic calculation using 33-group library. The results are shown in Table 4 and are consistent in terms of both void coefficients and enrichments with those calculated with KENO. The differences are considered to be caused by the difference in the energy group structure (238 groups vs. 33 groups) and difference in the self-shielding treatment. As seen in Tables 3 and 4, only Cores 4 and 6 have shown negative void coefficients all the way down to the voiding factor of 0.02. These two cores have water-to-fuel volume ratio of 1.0. In order to obtain more efficient conversion ratio, it could be preferable to use tighter fuel pin-pitch for the harder spectrum. However, tightening the pin pitch tends to increase the void coefficients.

Table 3. Void coefficients [pcm] of 10 m³ cores (cores 1-6) calculated by KENO-V.a.

Core Number	Volume [m ³]	Enrichment [wt% of Pu]	Voiding Factor				
			0.7	0.1	0.075	0.05	0.02
1	10	15.66	67.9±12.8	2530.3±13.4	2791.4±13.2	3088.5±14.3	3467.0±13.6
2	10	16.94	-402.6±12.9	-87.9±13.7	109.2±13.7	361.2±13.0	715.2±13.0
3	10	15.85	-113.0±13.1	1579.2±14.2	1774.3±13.4	2003.8±13.4	2292.0±13.5
4	10	17.15	-649.6±13.0	-1390.7±12.9	-1284.9±13.7	-1130.0±12.9	-909.4±12.9
5	10	16.08	-383.6±13.2	256.3±13.6	403.4±13.6	539.6±14.3	736.5±13.4
6	10	17.41	-927.6±11.4	-3005.7±12.6	-2997.8±12.6	-3011.6±12.6	-2946.9±12.6

Table 4. Void coefficients [pcm] of 10 m³ cores (cores 1-6) calculated by ERANOS2.2 using 33-group library.

Core Number	Volume [m ³]	Enrichment [wt% of Pu]	Voiding Factor				
			0.7	0.1	0.075	0.05	0.02
1	10	15.77	347.6	2162.1	2311.9	2456.1	2634.3
2	10	17.37	-257.3	57.9	147.4	252.7	396.9
3	10	16.07	184.9	1408.7	1504.4	1601.7	1728.4
4	10	17.74	-468.3	-1014	-982.8	-945	-887.6
5	10	16.43	-107.2	308.2	355.4	405.1	468.4
6	10	18.21	-724.0	-2335.5	-2380.1	-2421.4	-2463.3

Figure 5 shows void coefficients (voiding Factor = 0.02) and Pu enrichments as a function of H/D ratio. This figure well characterizes the relationships among void coefficients, Pu enrichments, core sizes, pin-pitches, and core shapes. Generally speaking, as reducing the core size and/or H/D ratio, the void coefficient decreases. The reducing of either parameter increases the surface-to-volume ratio of the core, which results in the increase of neutron leakage. In particular, the pancake-like core (small H/D) promotes more axial leakage while keeping the same core volume (similar to the design of sodium-cooled fast reactors). However, the increase of the surface-to-volume ratio is accompanied with the increase of Pu enrichment in order to have the same multiplication factor. Another basic approach to decrease the void coefficient is the use of wider pin-pitch. As seen in Figure 5, many of configurations with water-to-fuel

(W/F) ratio equal to 1 show the larger negative values of void coefficients compared to those of smaller W/F ratios. They could allow the addition of large size of blanket. However, the increase of enrichment is necessary to compensate the reactivity loss due to the decrease of the fuel volume. Also the spectrum will be softened, thus it is expected that the Pu conversion is less efficient than those having tighter pin-pitches.

(a) Void Coefficients vs. H/D Ratio (Error Bar = $\pm 1\sigma$)

(b) Pu Enrichment vs. H/D Ratio

Figure 5. Void coefficient and Pu enrichment as functions of H/D ratio.

2.3 Core with Axial and Radial Blanket

Now we start to add axial blanket to see changes in characteristics of the selected core configurations. Figure 6 shows the core configuration with axial blanket. As seen in this figure, the axial blanket has been added at the top of the core (as well as bottom of the core by reflection) while keeping the H/D ratios of the core region the same as those defined in Table 1. The blanket pin-pitch, pin diameter and clad thickness are kept as the same as those of the seed fuel. The blanket fuel temperature is set to 823.15 °K. Figure 7 shows relationships between void coefficients/Pu enrichments and the length of the axial blanket. It can be clearly observed that the void coefficient is very sensitive to the presence of axial blanket. For 7.5 m³ cores, adding only 1 cm of blanket costs void coefficient of more than 1000 pcm, and it is hard to keep negative unless reducing H/D and/or W/F ratios. On the other hand, the Pu content is not sensitive to the axial blanket. Less than 0.5% of enrichment change is necessary to keep k_{eff} of 1.02 for 5cm axial blanket.

Figure 6. Cylindrical core configuration with axial blanket.

(a) Void Coefficients vs. Axial Blanket Length

(Error Bar = $\pm 1\sigma$)

(b) Pu Enrichment vs. Axial Blanket Length

Figure 7. Void coefficient and Pu enrichment as functions of axial blanket length.

From the previous observation, it has been found that it is possible to add limited size of axial blanket at top and bottom of the core. However, it might be also possible to add axial blanket inside of the core (internal blanket). This could possibly promote more axial leakage of neutrons and thus lead to the negativity of the void coefficient. Figure 8 shows the core configuration with internal blanket. The same

conditions (i.e., pin-pitch, etc.) as those of the axial blanket apply to the internal blanket. The void coefficients and Pu enrichments as functions of internal blanket length are shown in Figure 9. As seen in this figure, the void coefficient is less sensitive to adding axial blanket inside of the core than cases with adding blanket at top and bottom of the core. However, the results indicate that the Pu enrichment is extremely sensitive to the addition of the internal blanket. Nearly 3% of enrichment change is necessary to add 10 cm of internal blanket while only 0.5% of change is required for adding the same size of blanket at top and bottom ($5 \text{ cm} \times 2$).

Figure 8. Cylindrical core configuration with internal blanket.

(a) Void Coefficients vs. Internal Blanket Length
(Error Bar $\pm 1\sigma$)

(b) Pu Enrichment vs. Internal Blanket Length

Figure 9. Void coefficient and Pu enrichment as functions of internal blanket length.

The last configuration we need to consider in this section is the radial blanket. We have selected only 7.5 m³ cores to analyze the effect of the radial blanket. Figure 10 shows the core configuration with radial blanket. Figure 11 shows the relationship between void coefficients/Pu enrichment and the radial blanket thickness. The results indicate that both Pu content and void coefficient are not sensitive to the addition of the radial blanket. The reason is that the axial neutron leakage dominates in the flat pancake-like core design. In this respect, the addition of radial blanket could be the promising way for the Pu conversion; however, the spectrum may not be hard enough to effectively produce Pu.

In summary, basic impacts of the addition of radial and axial blankets on the D₂O-cooled PWR core are:

1. The Pu content in the core is not sensitive to the addition of the axial blanket at top and bottom. However, the void coefficient is very sensitive to it.
2. The void coefficient is not sensitive to the addition of the internal blanket, however, the Pu content of the core is very sensitive to it since the internal blanket promotes axial leakage, and thus it is necessary to increase the enrichment of the core in order to compensate the loss of reactivity due to the axial leakage. More analyses will be done in Section 3.1.2 with burnup calculations.
3. Neither the Pu content nor void coefficient is sensitive to the addition of the radial blanket since the axial neutron leakage dominates in the flat pancake-like core design.

Figure 10. Cylindrical core configuration with radial blanket.

(a) Void Coefficients vs. Radial Blanket Thickness
For 7.5 m³ core, H/D=0.2, W/F=0.6 (Error Bar = $\pm 1\sigma$).

(b) Pu Enrichment vs. Radial Blanket Thickness
For 7.5 m³ core, H/D=0.2, W/F=0.6.

Figure 11. Void coefficient and Pu enrichment as a function of radial blanket thickness.

3. BURNUP CALCULATIONS

3.1 Burnup Calculations for the Evaluation of Axial Blanket Performance

3.1.1 Methodology

The burnup calculations have been performed based on the study of optimum core configurations contained in the previous section. For burnup calculations, we have selected 7.5 m³ core configurations having sufficiently large negative values of void coefficients at BOL (i.e., cores 11-15). The problem here is that it is not possible to perform burnup calculations using cylindrical geometry configurations used in the previous section since each individual nuclide density will be lost after the unit cell homogenization. In this respect, we need to use somehow explicitly modeled configuration. However, burnup calculations with Monte Carlo method using explicitly modeled whole core are extremely time consuming considering that we need to obtain statistically reliable tallies for each reaction rate. For this preliminary study, we only need some handy and simple models that give us reasonable estimates as quickly as possible. Therefore, we have decided to use 3-D hexagonal pin-cell geometry for burnup calculations, which is reasonable for evaluating the performance of axial blankets [13]. The model consists of hexagonal pin-cell geometry described in Section 2.2 with reflective boundary condition on all six radial surfaces and vacuum boundary condition on top and bottom (Figure 12). The fuel zone has been subdivided into 5-7 zones in order to taken into account the effect of axial burnup. We have utilized TRITON sequence in SCALE6.1 [11], which effectively couples multigroup KENO-VI with ORIGEN depletion module.

Figure 12. KENO-VI 3D hexagonal pin-cell model.

3.1.2 3D-Pin Burnup Results

The core average specific power has been set to 37 W/g, corresponding to that of standard PWRs, which could reach the average discharge burnup of 50 GWd/t by Equivalent Full Power Days (EFPD) of 1351 days. Assuming a 3-batch core management scheme, the average end of cycle (EOC) burnup, B_{EOC} , is then equal to 33.3 GWd/t. Thus, the reactor must be critical at B_{EOC} in order to have enough reactivity to reach the target burnup of 50 GWd/t. The calculations have shown that $\Delta k_{eff} (= k_{eff}^{3D-Pin} - k_{eff}^{RZ})$ is approximately equal to 1500 pcm. Therefore, the Pu enrichments of all cases shown in the Section 2 of

this report have been re-adjusted in order to have k_{eff}^{3D-Pin} of around 1.015 at B_{EOC} . This has significantly increased the Pu content and thus the void coefficient at BOL.

Figures 13 and 14 show the k_{eff} evolution for given core configurations. The statistical error of k_{eff} at each state (not shown in figures) is around 20 pcm. Table 5 presents the void coefficients between BOL and 50GWd/t, estimated by separate cylindrical core calculations with KENO-V.a, and ΔPu_f , which is defined as the relative difference between the final and initial fissile (i.e., ^{239}Pu and ^{241}Pu) masses after a given burnup:

$$\Delta Pu_f = \frac{M_{Pu_{fissile}}(50 \text{ GWd/t}) - M_{Pu_{fissile}}(BOL)}{M_{Pu_{fissile}}(BOL)} \times 100 \quad [\%]. \quad (3)$$

This value should be positive when the conversion ratio is more than one. The reactivity loss between the BOL and the target burnup of 50 GWd/t decreases as reducing W/F ratio, which can be observed in Figures 13 and 14 such that k_{eff} slope is lower for cores having smaller W/F. The reactivity loss is approximately 10% for W/F=1.0, 8% for W/F=0.6, and 7% for W/F=0.45. In all configurations, the required Pu enrichment in order to make the reactor critical at B_{EOC} is approximately 2-3% higher, and its void coefficient at the initial state is approximately 1500 pcm higher than that has been shown in Section 2, according to Table 5. Some configurations, Core 13 (W/F=0.45, H/D=0.2) and Core 11 (W/F=0.6, H/D=0.2), has positive void coefficients at BOL. Only Core 15 (W/F=0.45, H/D=0.15) remains negative values in void coefficient until 50 GWd/t. None of configuration has shown the positive value of ΔPu_f . The axial blanket at top and bottom of core seems to be more effective than the internal blankets. The reason for this observation is that the initial fissile Pu content of the seed fuel is high in configurations with internal blankets, thus it is difficult to compensate the net production of Pu by the similar size of blanket as the axial blanket, which requires less initial Pu content in the seed fuel. However, the utilization of the internal blanket could be possible to have higher conversion in heterogeneous designs of assembly or core by increasing the Pu content of its peripheral fuel pins or assemblies.

Figure 13. Evolution of k_{eff} until 50 GWd/t for core with (a) No Blanket, and (b) 1 cm Blanket at Top & Bottom.

Figure 14. Evolution of k_{eff} until 50 GWd/t for core with (a) 2 cm Internal Blanket, and (b) 4 cm Internal Blanket.

Table 5. ΔPu_f and Void coefficients [pcm] of 7.5 m³ cores determined by 3-D pin-cell models.

Blanket	W/F	H/D	Core Height (w/ blanket) [cm]	Initial Enrichment [wt%]	Void Coefficient [pcm]			ΔPu_f [%]
					At BOL	Near B_{EOC}	At 50 GWd/t	
No Blanket	1.0	0.2	72.556	20.59	-3763.7±12.2	-798.4±12.9	291.4±13.3	-12.000
	0.6	0.2	72.556	18.42	-259.7±10.6	2567.3±12.2	3438.3±12.3	-8.134
	0.45	0.2	72.556	17.40	341.4±11.4	2955.0±11.8	3740.6±12.3	-5.818
	0.45	0.175	66.376	17.76	-1391.7±11.1	1132.5±11.5	1850.0±12.2	-6.810
	0.45	0.15	59.894	18.03	-3995.8±11.7	-1451.9±12.0	-802.4±11.1	-7.624
1 cm Blanket at Top and Bottom	1.0	0.2	74.556	20.63	-2542.6±11.3	573.2±12.1	1640.7±12.7	-11.379
	0.6	0.2	74.556	18.39	746.4±10.7	3493.4±11.8	4381.5±11.8	-7.153
	0.45	0.2	74.556	17.45	1371.1±10.8	3783.8±11.5	4552.0±11.5	-4.849
	0.45	0.175	68.376	17.81	-174.5±11.3	2206.9±11.4	2922.5±10.9	-5.689
	0.45	0.15	61.894	18.11	-2376.2±11.0	-103.8±12.1	641.9±11.8	-6.473
2 cm Internal Blanket	1.0	0.2	74.556	21.22	-3448.6±11.7	-208.1±12.3	801.9±12.1	-11.943
	0.6	0.2	74.556	19.06	-183.8±10.3	2786.3±11.9	3761.2±11.4	-8.179
	0.45	0.2	74.556	17.94	395.7±11.0	3116.2±11.1	3926.8±10.7	-5.790
	0.45	0.175	68.376	18.33	-1391.4±11.1	1366.8±11.6	2178.9±12.5	-6.646
	0.45	0.15	61.894	18.64	-3824.9±11.7	-1121.4±11.8	-257.7±11.7	-7.425
4cm Internal Blanket	1.0	0.2	76.556	21.93	-3031.0±11.2	327.8±12.1	1343.3±13.4	-11.693
	0.6	0.2	76.556	19.62	-40.4±10.9	2985.5±11.7	3989.4±12.4	-7.935
	0.45	0.2	76.556	18.53	420.9±10.5	3280.3±10.8	4111.7±12.2	-5.795
	0.45	0.175	70.376	18.96	-1251.8±11.7	1596.6±12.4	2493.4±12.1	-6.667
	0.45	0.15	63.894	19.32	-3624.7±11.3	-736.9±11.6	145.7±12.9	-7.324

So far we have compared 3D pin-cells with three types of axial blanket, namely 1 cm axial blanket, 2 cm internal blanket, and 4 cm internal blanket. For the purpose of comparative study, we further subdivide these types of rod into four categories. Those are:

1. “No Blanket” core (the core without axial blanket),
2. “Long” core (the core with axial blanket, the same configuration used to calculate results in Figures 13, 14 and Table 4),
3. “Short” core (the core with axial blanket, the total axial height is the same as “No Blanket” core, but the fuel enrichment is the same as that of “Long” core), and
4. “Less”^a core (the same configuration as “Short” core, but the initial Pu enrichment in the fuel is the same as “No Blanket” core).

Figure 15 describes axial configurations of these 3D pin-cells for clarification.

Figure 15. Axial configuration of 3D-pin-cell models.

Figures 16 and 17 show burnup dependence of void coefficients for each 3D pin-cell model defined in Figure 15. The “No Blanket” core with W/F=0.6 can only sustain the negativity of the void coefficient until the burnup reaches ~5 GWd/t while that of W/F=1.0 has negative void coefficients up to ~45 GWd/t. The addition of the axial blanket also significantly increases the void coefficient even if we match the core height to that of the “No Blanket” core. This situation can be altered if the internal blankets are used. The direct addition of the internal blanket (i.e., “Long” core) slightly increases the void coefficient. However, if the core height is lowered to match the “No Blanket” core, it can decrease the void coefficient since the addition of internal blanket promotes the axial neutron leakage. The “Short” and “Less” cores with W/F=1.0 keeps negative void coefficients until the target burnup of 50 GWd/t. Yet the important point here is that we have reduced the size of axial height, which means we have also reduced

^a This footnote was made in order to avoid confusion. The name “Less” was chosen since this model has less axial height and Pu content than the “Long” core. Only one exception is in 1cm axial blanket with W/F=0.6, in which the “No Blanket” Pu content is slightly higher than the “Long” core.

the reactivity. Figure 18 presents the burnup dependence of Pu content within internal blankets. These figures prove that the slight change of Pu content within the fuel is not sensitive to the Pu conversion in blanket. From the observations made in this section of the report, the inclusion of the internal blanket can be the effective option when it is modeled with highly heterogeneous arrangement of fuel pins and/or assemblies. It is important to note that the inclusion of the internal blanket itself introduces decoupling of the axial core power profile, which could produce high local power peaking and unstable transient [2]. However, this can be mitigated by the heterogeneous arrangement of seed fuel and internal blanket assemblies.

Figure 16. Burnup dependence of void coefficients for $W/F=0.6$, $H/D=0.2$ (Error Bar = $\pm 1\sigma$)

Figure 17. Burnup dependence of void coefficients for $W/F=1.0$, $H/D=0.2$ (Error Bar = $\pm 1\sigma$).

Figure 18. Burnup dependence of Pu content within internal blankets.

3.2 Burnup Calculations for the Evaluation of Radial Blanket Performance

3.2.1 Methodology

For the evaluation of radial blanket performance, we have come up with a fairly simple burnup scheme utilizing the existing KENO models that can take into account the radial spectrum effect. This scheme is shown in Figure 19. The calculation starts from the criticality calculation using the RZ model given in Figure 20. There is no axial blanket in this model. The core region is divided into 5 axial and radial burnup zones such that all zones have the same volume. The blanket zone, which has radial thickness of 10 or 20 cm, is only axially divided into five zones. The specific power of each radial burnup zone is calculated based on the radial power distribution obtained from the RZ calculation. The calculated radial specific power is used for the input of 3D pin-cell burnup calculation for each radial zone. After the 3D pin burnup calculations for only one time step, 230-250 new nuclide compositions at each burnup zone are transferred to the RZ criticality calculations for the next time step. This process is repeated until the final time step.

Figure 19. Procedure of radial burnup calculations

Figure 20. Radial zones arranged for the burnup calculations

The core average specific power has been set to 37 W/g. For the verification of this methodology, the radial profiles of specific powers are plotted in Figures 21-23. As seen in these figures, initially cosine shaped power profiles are flattened as the burnup proceeds, which clearly makes sense that the radial burnup effects are successfully captured at each time step. In 10cm blanket zone the specific power is increased from ~2% to ~15% of the core average specific power between 0 and 50 GWd/t, while in 20cm blanket, it is increased from ~1% to ~6%.

Figure 21. Radial specific power profile (w/o radial blanket)

Figure 22. Radial specific power profile (10 cm radial blanket)

Figure 23. Radial specific power profile (20 cm radial blanket)

3.2.2 Radial Burnup Results

Figure 24 shows the evolution of k_{eff} until 50 GWd/t obtained from radial burnup calculations. Here “Radially Flat Core” means the core without radial burnup zones and corresponds to “No Blanket” core presented in Section 3.1.2 for the 3D-pin calculations. The only difference is that here k_{eff} are evaluated by RZ criticality calculations. Thus k_{eff} 's presented here are approximately 1500 pcm lower than those presented in Figure 13. As seen in these figures, the reactivity losses of cores with radial burnup zones are slightly higher than that of the radially flat core.

Table 6 shows void coefficients between BOL and 50 GWd/t and the relative difference of fissile Pu content, ΔPu , defined by Eq. (3). The void coefficients of the core with 5 radial zones are very close to those of the radially flat core. The same observation can be made for ΔPu . In this respect, the 3D pin-cell burnup calculation alone can essentially predict the average core behavior very accurately. The addition of the radial blanket slightly increases the void coefficients although it is not significantly sensitive as discussed in Section 2.3. The radial blanket certainly helps to increase the fissile Pu content. Figure 25 shows the burnup dependence of fissile Pu contents in radial blanket zones. As expected, the tighter pin-pitched core (small W/F ratio) produces more Pu than the wider one since the former has harder spectrum even in the radial blanket zone located outside of the core. However, 10 cm- and 20 cm- blankets produce fissile Pu in almost the same rate. This means that the addition of thicker radial blanket in the outer core region is not effective for increasing the Pu conversion ratio.

Figure 24. Evolution of k_{eff} until 50 GWd/t for radial burnup calculations (Error Bar = $\pm 1\sigma$).

Table 6. ΔPu_f and Void coefficients [pcm] of 7.5 m³ cores determined by radial burnup calculations.

W/F & H/D	Model	Radial Blanket [cm]	Initial Enrichment [wt%]	Void Coefficient [pcm]			ΔPu_f [%]
				At BOL	Near B_{EOC}	At 50 GWd/t	
0.6 & 0.2	Radially Flat (3D-Pin)	0	18.42	-259.7±10.6	2567.3±12.2	3438.3±12.3	-8.134
	5 Radial Zones	0	18.42	-265.7±11.1	2850.5±12.0	3637.2±12.1	-7.801
	5 Radial Zones	10	18.35	-190.5±10.3	3042.2±10.8	3915.0±11.2	-6.413
	5 Radial Zones	20	18.35	-105.2±11.5	3169.6±11.4	4030.3±11.3	-6.354
1.0 & 0.2	Radially Flat (3D-Pin)	0	20.59	-3763.7±12.2	-798.4±12.9	291.4±13.3	-12.000
	5 Radial Zones	0	20.59	-3780.0±10.9	-436.1±12.5	481.4±12.5	-11.594
	5 Radial Zones	10	20.54	-3662.2±11.7	-104.0±11.7	832.4±12.9	-10.328
	5 Radial Zones	20	20.55	-3545.4±10.8	57.0±12.5	1069.7±12.0	-10.230

Figure 25. Burnup dependence of the fissile Pu content (²³⁹Pu+²⁴¹Pu) within the radial blanket of 7.5 m³ core.

3.3 Burnup for Simple 3D Assembly Models with Seed and Blanket Fuel Pins

The seed-blanket assembly designs had been studied by Radkowsky [4] and Hibi [3] in D₂O moderated PWR cores in order to achieve the higher conversion. This assembly design is constituted by arranging a bundle of blanket fuel pins around seed fuel pins or vice versa. The combination with axial zoning of seed and blanket fuels could lead to more effective conversion and reduce the void coefficient. With the limited time allowed in FY12, we have selected very few cases to perform the analysis of heterogeneous assemblies. The design of simple seed-blanket assembly model for KENO-VI calculation is shown in Figure 26. The model is based on the 3D-pin model having W/F ratio of 0.45 and H/D ratio of 0.15 given in Section 3.1. There are total of 217 fuel pins. Approximately a third of fuel pins at the outer ring of the assembly (66 pins) are chosen to be internal blanket fuel pins, in which blanket is axially sandwiched by seed fuel pins. The rest of fuel pins inside of the assembly are seed fuel pins consisting of the seed fuel zone and axial blanket at top and bottom. The fuel bundle is enclosed by stainless steel (SS) wrapper radially and 20 cm D₂O shield at top and bottom. The reflective boundary conditions are applied on all six radial surfaces of the assembly whereas the vacuum boundary conditions are used at top and bottom surfaces. For burnup calculations with TRITON, a total of 49 burnup zones are created by dividing the radial and axial fuel zones into seven rings and seven segments, respectively. There are total of five assembly burnup calculations performed. Those are: (a) Core I – no blanket and the same Pu enrichment for both types of fuel pins, (b) Core II – 1 cm axial blanket at top & bottom, 10 cm internal blanket, and the same enrichment for both types of fuel pins, (c) Core III – the same configuration as Core II, but lower Pu enrichment for Seed Fuel 2, (d) Core IV – 2 cm axial blanket at top & bottom, 20 cm internal blanket, and the same enrichment for both types of fuel pins, and (e) Core V – the same configuration as Core IV, but lower Pu enrichment for Seed Fuel 2. The void coefficients are evaluated at burnup states of interest by voiding the 3D assembly model, which is different from 3D pin-cell burnup cases in Sections 3.1 and 3.2 that void coefficients are evaluated by R-Z core calculations. Therefore the void coefficients obtained in this section are expected to be higher than those obtained in previous sections due to the absence of the radial leakage.

Table 7 shows the relative difference of fissile Pu contents, ΔPu , defined by Eq. (3) and void coefficients evaluated at BOL, near B_{EOC} , and 50 GWd/t. Figure 27 presents the k_{eff} evolution until 50 GWd/t of each case. The Pu enrichment of each case has been adjusted based on the prior experience obtained by 3D pin-cell calculations with W/F ratio of 0.45 and H/D ratio of 0.15. However, as seen in Figure 27, k_{eff} is significantly lower than 1.015 around B_{EOC} of 33 GWd/t. This could be primarily caused by the neutron capture within the SS assembly wrapper. Therefore, the assembly wrapper of this type of reactors should use the material which is transparent to the neutron, or even it is not necessary to be equipped so that there is enough excess reactivity to be critical at B_{EOC} with less Pu enrichment. The ΔPu 's presented in Table 7 reveals that the addition of blankets increased the values of ΔPu in negative direction, which means it decreased the conversion ratio. This occurs due to the higher initial enrichment associated with the addition of internal blankets. However, there are some promising signs if the enrichment variation is introduced between two types of pin-cells. The studies performed in Section 3.1.2 based on 3D pin-cell models have shown that the initial enrichment of the seed fuel is less sensitive to the Pu production rate within the internal blanket (Figure 18). Thus, the idea is that there could be improvement in conversion ratio if the enrichment of seed fuel within the internal blanket fuel pin is lowered, as well as adjusting the enrichment of inner fuel bundle to have enough excess reactivity. As seen in Table 7, there is slight improvement in ΔPu of Cores III and V compared to their counter parts, Cores II and IV, respectively. To further increase the conversion ratio while keeping the negative void coefficient, the assembly must be highly heterogeneous, or it must be considered in the core level heterogeneity such as the checkerboard arrangement of seed assemblies and seed-blanket assemblies.

Figure 26. Radial and axial details of the simple assembly model for KENO-VI.

Table 7. ΔPu_f and Void coefficients [pcm] determined by assembly burnup calculations.

Core Name	Initial Pu Enrichment [wt%]		Blanket Axial Length [cm]		Void Coefficient [pcm]			ΔPu_f [%]
	Seed Fuel 1	Seed Fuel 2	Blanket A	Blanket B	At BOL	Near B_{EOC}	At 50 GWd/t	
Core I	19.95	19.95	0	0	-2269.7 $\pm$ 27.2	-266.8 $\pm$ 30.9	563.5 $\pm$ 32.3	-11.891
Core II	21.35	21.35	10	1	-1645.1 $\pm$ 30.3	365.3 $\pm$ 30.9	772.5 $\pm$ 35.1	-12.084
Core III	22.08	19.00	10	1	-1548.3 $\pm$ 29.9	408.0 $\pm$ 30.9	1140.9 $\pm$ 32.4	-12.036
Core IV	23.15	23.15	20	2	-810.5 $\pm$ 28.1	1029.4 $\pm$ 31.0	1826.5 $\pm$ 31.6	-12.456
Core V	24.08	19.00	20	2	-595.0 $\pm$ 28.8	1223.1 $\pm$ 29.7	1984.4 $\pm$ 31.8	-12.058

Figure 27. Evolution of k_{eff} until 50 GWd/t for assembly burnup calculations (Error Bar = $\pm 1\sigma$).

4. CONCLUSIONS

This report presented the analyses of the U-Pu fueled D₂O cooled PWRs focusing primarily on small sized cores (less than 10 m³) in order to obtain fundamental design characteristics of this type of reactors, aiming at high Pu conversion ratio and negative void reactivity. The SCALE6.1 code system was utilized to perform a series of Monte Carlo based criticality and burnup calculations.

The optimum core size and configuration were investigated by means of a series of criticality calculations with simple cylindrical core models. The results had shown that the void reactivity coefficients tend to be negative in smaller sized cores (5-7.5 m³), in particular those having flat pancake like configuration (similar to FBR design). The Pu enrichment in the seed fuel was not sensitive to the addition of the axial blanket outside of the core while the void coefficient was increased significantly. Contrarily, the void coefficient was not sensitive to the addition of the internal blanket; however, the Pu enrichment of the core was very sensitive to it. Neither the Pu enrichment nor void coefficient was sensitive to the addition of the radial blanket since the axial neutron leakage dominated in the flat pancake-like core design.

Burnup calculations were performed in order to evaluate the performance of axial and radial blankets. For the estimation of the performance of the axial blanket, the burnup calculations were performed using 3D single pin-cell model. The results showed that the addition of axial blanket at the top and bottom of the core slightly increased the net Pu content compared to that of the core without blanket; however, the void coefficients were significantly increased and became positive before the target burnup of 50 GWd/t. The direct use of internal blankets did not result in an increase in the conversion ratio effectively compared to top and bottom axial blankets since the use of internal blanket required more initial Pu content in order to have enough excess reactivity. However, they allow reducing the void coefficient by shortening the size of fuel pin. Also the study had shown that the initial enrichment of the seed fuel was less sensitive to the Pu production rate within the internal blanket. The burnup effect of radial blanket was investigated by means of an iterative approach between the cylindrical core model and 3D pin-cell burnup calculations. Both initial Pu content and void reactivity coefficient were not sensitive to the addition of the radial blanket, and it was able to increase the net production of Pu. However, the addition of thicker radial blanket in the outer core region was not effective for increasing the Pu conversion ratio. Finally, burnup calculations with simple 3D assembly models were performed in order to investigate the performance of the seed-blanket assembly. The assembly model was determined based on the tightest pin-pitch and shortest core configuration used in 3D pin-cell calculations (W/F ratio = 0.45 and H/D = 0.15). The results showed that none of cases increased the net Pu production effectively. However, slightly higher net Pu production was observed those having lower Pu enrichment in the seed fuel within internal blanket fuel pins compared to those having the same Pu enrichment in all seed fuels.

Most of the efforts in this work had been spent for identifying the core parameters needed for the high Pu conversion and negative void reactivity by simplified calculations; however, we could not cover all possible configurations within the limited time allowed in this fiscal year. Unfortunately none of configuration investigated in this report had a conversion ratio greater than 1.0. The reason is that we initially limited the selected configurations to those having negative void coefficients. Based on the studies in this report, the easiest way to achieve high conversion ratio is to add axial blankets at the top and bottom of the core. However, the consequence will be significant increase in the void coefficient. The optimum core design could be highly heterogeneous, and as such cannot be determined by simple fuel pin or assembly models. Thus, there is a strong incentive to perform high dimensional whole core designs as future tasks. The conservative but fast and integrated approach to perform the whole core burnup calculation is to utilize existing deterministic full-core simulator suits such as CASMO-SIMULATE [14, 15]. Thanks to the steady improvement of computational environment, the full core Monte Carlo burnup calculations for RBWR cores were recently simulated with the thermal-hydraulic coupling by Feng and Ganda [10] using MCODE [16] and SCALE [11]. Therefore, it is also interesting to pursue the robust simulations based on Monte Carlo method.

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