

Ranking of Aluminium Composite Materials for Use as Neutron Absorber Inserts in Spent Fuel Pools

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Abstract

A number of spent fuel pools at nuclear power stations that have been operating since the mid 1980s or earlier are gradually approaching their full capacity. This puts pressure on the nuclear facility to develop strategies to increase the storage space of the spent fuel pool if untimely shut down is to be avoided. One of the methods that can be employed is to insert neutron-absorbing materials in the spent fuel pool with a view to reducing the number of thermal neutrons which cause fission. This will subsequently reduce the k_{eff} of the system and permit a higher fuel storage density.

This paper presents an evaluation of the suitability of the material used as neutron absorber inserts (or absorber inserts for short) and ranks several aluminium composite materials for use as absorber inserts on the basis of their effectiveness in decreasing the k_{eff} of the system, thereby recovering some of the storage space consumed as a result of over-conservatism.

Key words

neutron absorber inserts, burnup credits, aluminium composite material, spent nuclear fuel, end-effect, borated steel, boraflex

1.0 Introduction

Many nuclear power stations commissioned before the mid-1980s are gradually running out of storage space in the spent fuel pool, putting the facilities at risk of shutting down prematurely if a solution to preserve storage space is not in place in time. Although the application of burnup credit has been proven [1, 2, 7] to have a significant impact on the reduction of k_{eff} and the corresponding recovery of extra storage space associated with over-conservatism in calculations, there is still much uncertainty regarding its acceptability.

While most nuclear regulators have approved the application of burnup credit of Actinides nuclide set for use in casks [1, 7], few have approved *Actinide + Minor Fission Products* and *Actinides + Principal Fission Product* nuclide sets. This further complicates the problem in that had either of these sets been approved, the operator of a nuclear facility would have had to acquire casks designed for the range of k_{eff} obtainable when credit for burnup of that specific nuclide sets is taken into account [3]. In that case most of the spent fuel assemblies in the spent fuel pool, which have to wait for an out-of-reactor cooling period of 10 years to meet the cask loading requirement, would have met it much earlier and would therefore have

been transferred into the storage casks earlier, thereby reducing the number of fuel assemblies in the spent fuel pool.

The challenge associated with the decrease in storage capacity is further exacerbated by the fact that the spent fuel pool has its own loading requirements to comply with. These are defined by its burnup credit loading curve [1] which, depending on the nuclide sets used in burnup credit analyses, can either allow for much more densely packed fuel assemblies or sparsely packed assemblies. Therefore, as a result of the over-conservatism associated with a *fresh fuel approach* and the resulting ineffectiveness in conserving storage space there is a continuous decrease in the storage space available.

To increase the storage capacity of the spent fuel pool, a number of aluminium composite materials have been analysed with the aim of determining which of them would be most effective in decreasing the k_{eff} when used as an absorber insert, consequently resulting in a saving of storage space. In addition to evaluating the composition of the neutron absorber material, the study on which this paper is based also investigated the most optimum area on the fuel assembly for locating the absorber insert which would result in the highest Δk_{eff} and a corresponding saving in the spent fuel pool storage space.

The effectiveness of the absorber inserts is a function of a combination of the *composition* of the composite material and the *location* of the inserts in the fuel assembly. To obtain maximum benefit from the inserts they must be located in the region of the fuel assembly that has the highest neutron flux, where they will reduce the number of thermal neutrons that cause fission and thereby reduce the k_{eff} .

2.0 Methodology

Three aluminium composite materials were studied, BORAFLEX (1.7 g/cm³), AA1100 (2.71 g/cm³) and ALCAN (2.76 g/cm³),¹ with their respective relative densities given in brackets. The selection of these materials was based on similar studies that have been conducted previously [4-6]. The materials were further divided into their respective subdivisions, depending on whether their composition contained Fe or Si (see Table 1).

The analyses were based on a single fresh fuel assembly with a uniform initial enrichment of 4.4 wt%. The fuel assembly under discussion is a 17X17-25² PWR fuel assembly consisting of 264 fuel rods, with an active and a total height of 3.6571 m and 4.06337 m, respectively [1]. The reason for selecting fresh fuel was that it provides the most conservative k_{eff} values where the results would envelop cases for similar calculations where burnup credit is taken into account. Since the fuel assembly had uniform enrichment, it was expected that it would result in an uneven distribution of the neutron flux along the length of the fuel assembly, which would subsequently give rise to an end-effect [2, 7, 12]. This is of particular concern in the storage of fresh or underburned fuel assemblies, since it implies that fuel assemblies should be stored further apart from one another to prevent interaction than would have otherwise been the case [3, 12].

The calculations were performed using KENO-VI, a module of SCALE 6.1.3 computer code using v7-238 neutron cross-section library. The neutron sample size consisted of 10100 neutron generations and 10000 neutrons per generation, skipping 100 neutron generations [8].

¹ The density of ALCAN when B₄C is added is 2.8 g/cm³.

² 25 non-fuel rods in the fuel assembly.

Table 1: Chemical composition of composite material used as absorber inserts

Elements	AA100 UNS A91100 Temper O (%)	Boral Metal Matrix Material Spec (%)	ALCAN Metal Matrix Material Spec (%)	ALCAN 15.3% (%)	ALCAN 15.9% (%)
Al	99 min	99 min	99 min	97.214059	97.00698
Si	0.95 max	1.00 max	0.45 max	0.446691	0.461375
Fe					
Cu	0.05–0.20	0.05–0.20	0.05–0.20	0.1293053	0.130131
Mn	0.05 max	0.05 max	0.05 max	0.011755	0.01183
Zn	0.10 max	0.10 max	0.10 max	0.011755	0.01183
Mg			0.05	0.011755	0.01183
Ti			1.00-2.5	2.1746797	2.366024
				100	100
B4C				15.30	15.90

3.0 Design of the Neutron Absorber Inserts

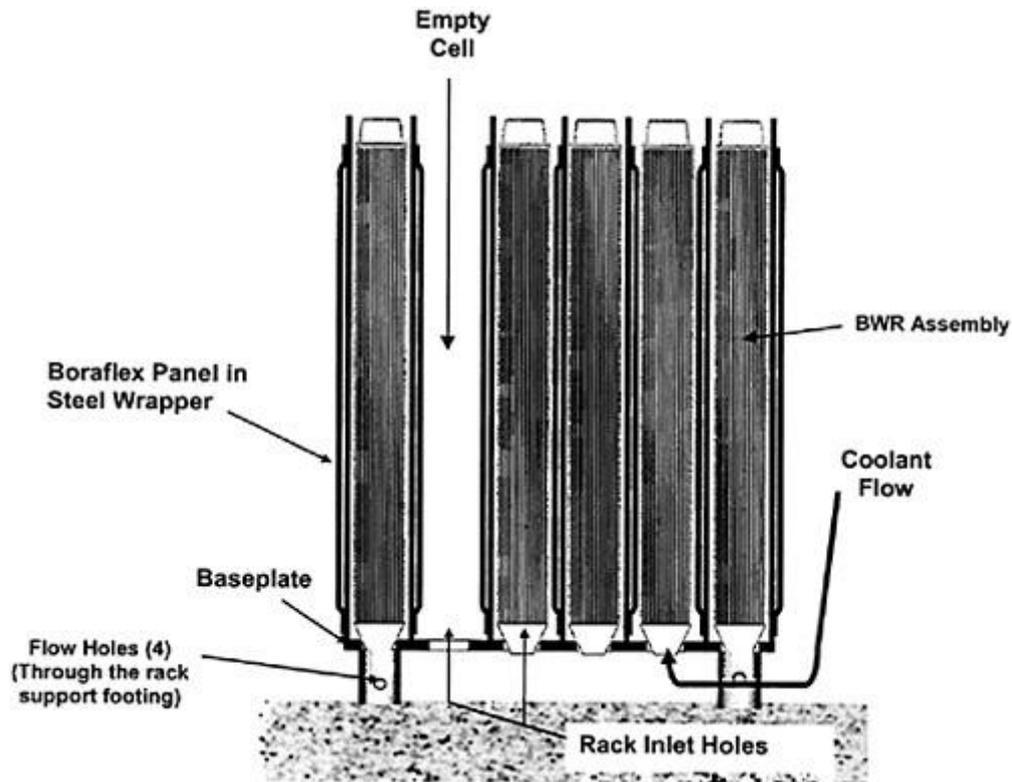


Fig. 1: Boraflex as an absorber insert [9]

The positioning of the absorber inserts on the fuel assembly is based on the need to find the optimum area in the fuel assembly where the highest decrease in the k_{eff} relative to the bounding reference case will result (which is the k_{eff} of fuel assembly in water that is not shielded by any neutron absorbing material). This will subsequently result in freeing up some of the empty cells in the spent fuel pool, as indicated in Figure 1. Three main areas of the fuel

assembly where the inserts could be placed were assessed: 1) around the entire fuel assembly with absorber inserts forming *the basket* into which the fuel assembly is placed; 2) at the top and bottom of the fuel assembly to reduce the *end-effect*; and 3) in the *central instrumentation* tube. These will be discussed in detail in the following subsections:

3.1 The Basket Design

Central to the basket design is an assumption that when a fuel assembly is transferred from the reactor core to the spent fuel pool at the end of the fuel cycle, it goes into a flask made up of the absorber insert and is completely separated and shielded from other fuel assemblies, thereby yielding the expected decrease in k_{eff} . Three alternative methods for attaching the absorber insert in the fuel assembly were investigated:

- Case 1: In the first case, the original material composition of the basket was replaced with that of the absorber inserts indicated in Table 1.

In the second and third cases, the original thickness of the basket was divided into two layers, or regions as is often referred to in the KENO terminology, as follows:

- Case 2: In this case, the inner region, which is the region closest to the fuel assembly, was replaced with the composition of the absorber insert as indicated in Figure 2. In the outer region, the borated steel composition was kept the same and the two regions were separated by a vacuum layer.
- Case 3: In the third case, the inner region was made up of a vacuum, which was encased by the borated steel and the absorber insert was placed on the outside, as shown in Figure 3.

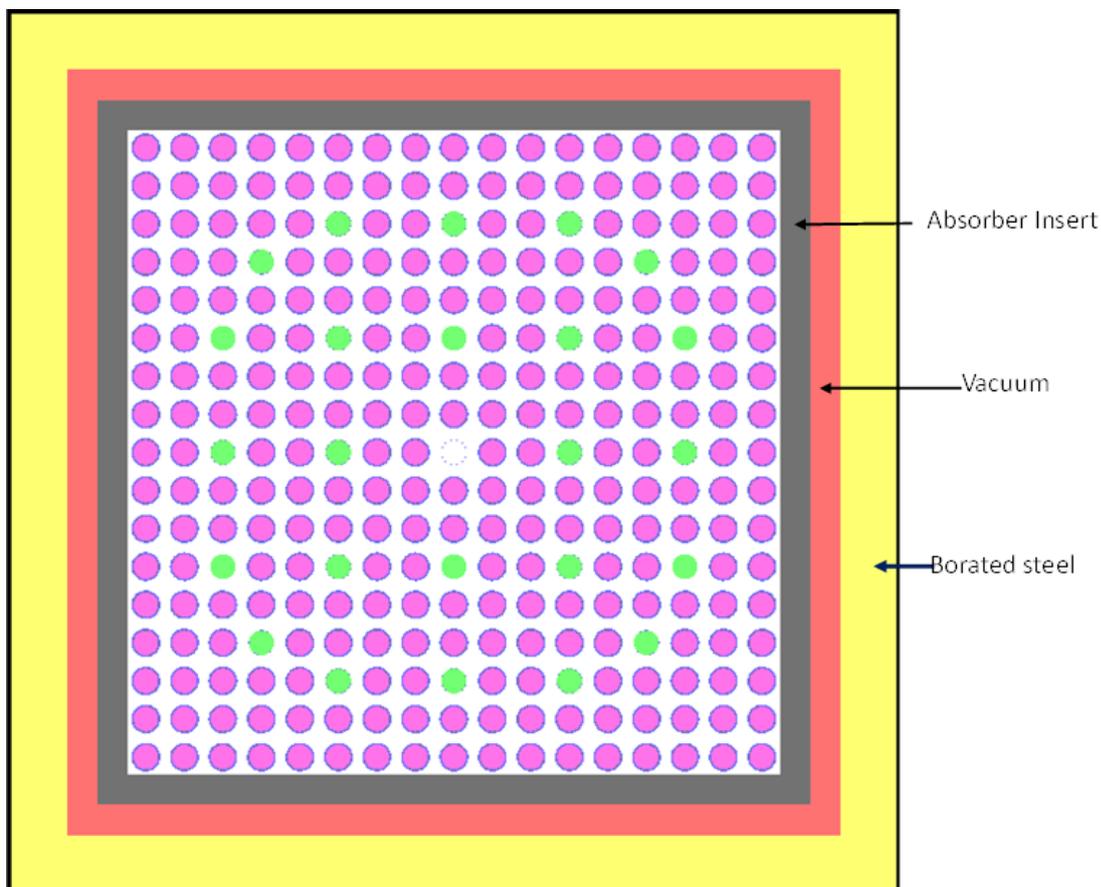


Fig. 2: Neutron absorber insert inside the fuel assembly flask

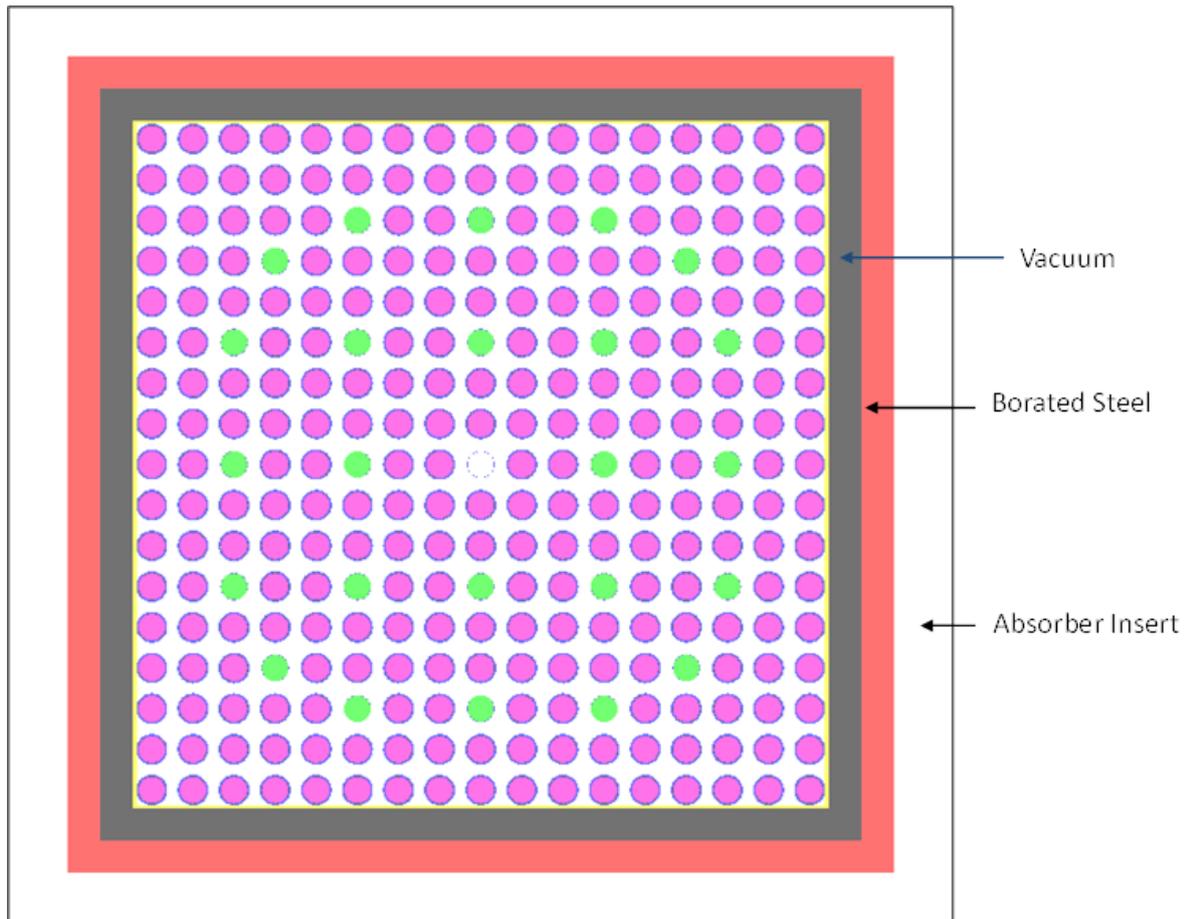


Fig. 3: Neutron absorber insert outside the fuel assembly flask

3.2 The End-Effect Design

The rationale for placing the absorber inserts at the top and bottom of the fuel assembly is based on the fact that, owing to the uniform enrichment of the fuel assembly and the uneven distribution of the neutron flux in the core, the fuel assembly has an *axial* and a *radial profile* resulting from the high nuclear reaction density occurring in the middle section of the fuel assembly, and much lower reaction densities in the top and bottom sections. It is therefore important that when fuel assemblies are stored, provision is made for extra storage space to prevent neutrons from one fuel assembly interacting with adjacent fuel assemblies and in so doing cause a nuclear criticality incident [3]. Thus, to minimise the extent of the end-effect on the fuel assembly, an absorber insert is placed at the top and bottom of the fuel assembly to cover its entire length [1].

In this design, the model will introduce three additional regions in addition to the reference case in order to make provision for the top and bottom sleeves of the design. Region 5 refers to the top sleeve, ranging from 76.1 to 201.1 cm, region 6 to the bottom sleeves ranging from -135.81³ to -185.81 cm and, finally, region 7 which is the global region that envelops the entire fuel assembly. Two scenarios were investigated: in scenario 1, region 4 of unit 4 was filled with water, as shown in the excerpt of the KENO-VI model indicated by Figure 4 and also by the schematic diagram shown in Figure 5. In scenario 2, the same region was filled

³ In this model 0, i.e. zero, is near the centre of the fuel assembly, the highest part being at 201.1 cm and the lowest part at -185.81 cm.

with borated steel and the results of the two scenarios were compared to other results summarised in Appendix 1.

com="complete fuel assembly"

cuboid 1 10.55 -10.55 10.55 -10.55 185.81 -185.81

cuboid 2 10.66 -10.66 10.66 -10.66 185.81 -185.81

cuboid 3 11.66 -11.66 11.66 -11.66 185.81 -185.81

array 1 1 place 9 9 1 0 0 0

cuboid 4 14.5 -14.5 14.5 -14.5 201.1 -185.81

cuboid 5 15.5 -15.5 15.5 -15.5 201.1 76.1

cuboid 6 15.5 -15.5 15.5 -15.5 -135.81 -185.81

cuboid 7 15.5 -15.5 15.5 -15.5 201.81 -185.81

media 5 1 2 -1 vol=126717.8

media 0 1 3 -2 vol=783422.8

media 8 1 4 -3 vol=2522055

Media 8(H₂O)
inside region 4

media 19 1 5 -4

media 19 1 6 -4

Media 19 (Boraflex_fe): Absorber inserts at the top and bottom of fuel assembly

media 8 1 7 -5 -6 -4

boundary 7

end geometry

global unit 4

Fig. 4: Excerpt of unit 4 of the end-effect design

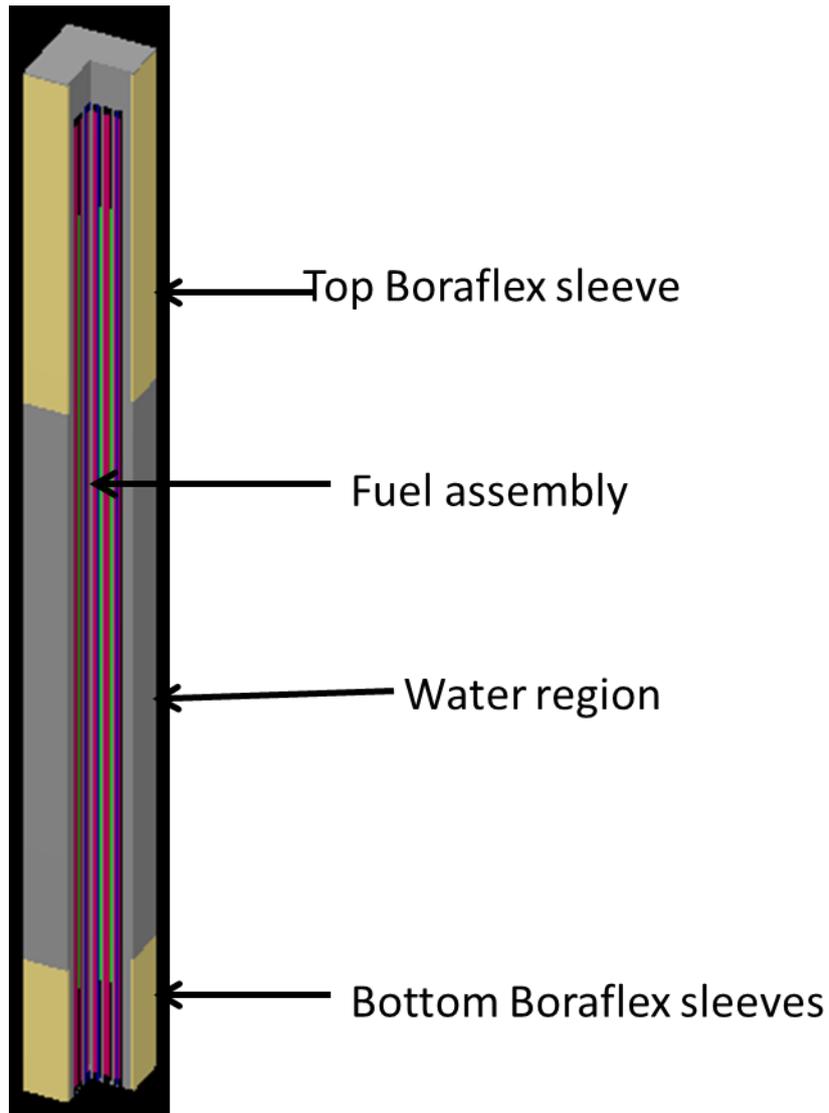


Fig. 5: Boraflex sleeves at the top and bottom end of the fuel assembly

3.3 Central Instrumentation Designs

In this design, two scenarios were investigated. In the first scenario the neutron absorber insert (media 21 in Figure 6) was pushed down into the instrumentation tube like a cord or a thread and had no cladding of its own. The schematic diagram of its cross section is shown in Figure 7.

com="instrumentation tube"

cylinder 1 0.39 182.88 -182.88

cylinder 2 0.395 185.68 -185.68

cylinder 3 0.4095 185.68 -185.68

cylinder 4 0.418 185.68 -185.68

cuboid 5 0.63 -0.63 0.63 -0.63 201.1 -185.81

media 21 1 1 vol=5395.254

media 2 1 2 -1 vol=312.3727
 media 8 1 3 -2 vol=10811.92
 media 2 1 4 -3
 media 8 1 5 -4
 boundary 5

Fig. 6: Excerpt of KENO VI model of the instrumentation tube showing the location of the neutron absorber (media 21)

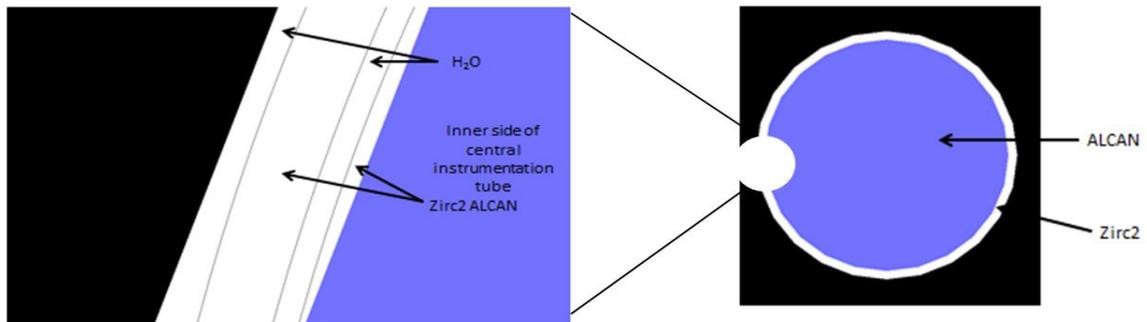


Fig. 7: Neutron absorber insert as a cord in the central instrumentation tube

In the second scenario, the absorber material was covered with its own zirc2 cladding material which, when viewed in the KENO VI model, media 21, is sandwiched between two cladding materials on either side, hence the name *sandwich* as shown in Figure 8. The schematic representation of this is shown in Figure 9.

Cylinder 1 0.4095 182.88 -182.88
 cylinder 2 0.416 185.68 -185.68
 cylinder 3 0.417 185.68 -185.68
 cylinder 4 0.418 185.68 -185.68
 cuboid 5 0.63 -0.63 0.63 -0.63 201.1 -185.81
 media 8 1 1 vol=5395.254
 media 2 1 2 -1 vol=312.3727
 media 21 1 3 -2 vol=10811.92
 media 2 1 4 -3
 media 8 1 5 -4
 boundary 5
 global unit 4

Figure 8: Excerpt of KENO-VI model where medial 21 is sandwiched by media 2 on either side.

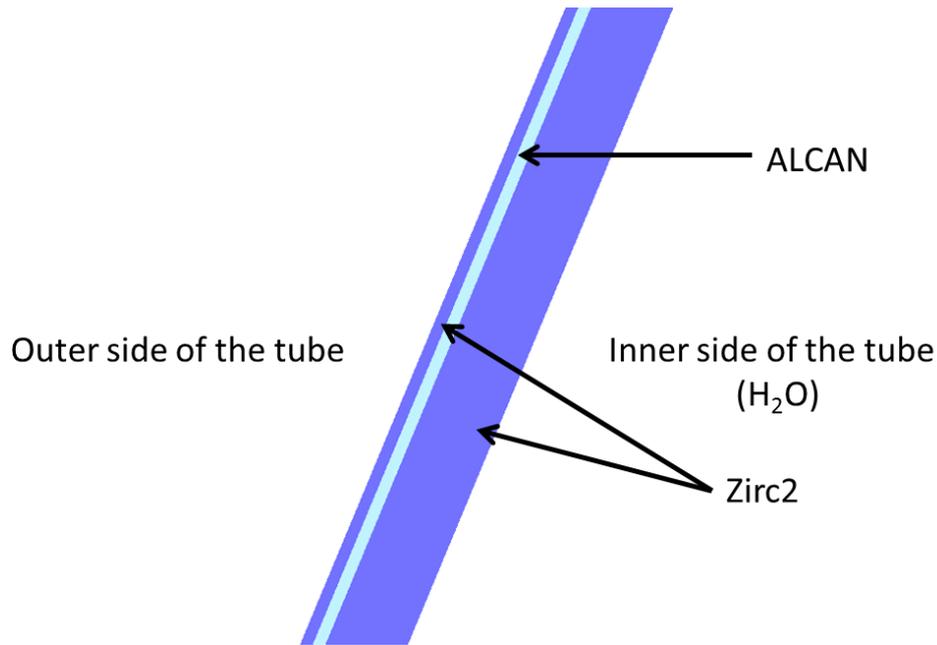


Fig. 9: Pictorial illustration of absorber inserts sandwiched by zirc2 cladding

4.0 Results

The results indicate that changing the position of the absorber insert while keeping the chemical composition the same has a much greater effect in decreasing the k_{eff} of the system than the other way around.

Of all designs, the basket designs, irrespective of the variation under consideration, have the greatest effect in decreasing the k_{eff} of the system. The advantage of these designs over other designs is that the absorber insert covers the fuel assembly completely, thus providing a very effective neutron shielding jacket around the fuel assembly which reduces the escape or ingress of neutrons from other fuel assemblies, subsequently resulting in the highest Δk_{eff} based on a calculation using Eq 1[2].

$$\Delta k_{eff} = \text{Bounding } k_{eff} - \text{Best-estimate } k_{eff} \text{ value} \quad \text{Eq 1}$$

$$\Delta k_{eff} / k_{eff} \times 100\% \text{ where } k_{eff} \text{ is the best-estimate } k_{eff} \text{ value}$$

where the best-estimate k_{eff} value is the k_{eff} value when the absorber insert forms part of the fuel assembly shielding material. On the effect of material composition on the k_{eff} , it was observed that within the same design some variations of the basket designs had higher or lower $\% \Delta k / k_{ref}$ than others, depending on the material that the neutrons interacted with first. When the three variations of the basket design were compared, it was observed that

- the largest decrease in k_{eff} was obtained when the composition of borated steel in the model was replaced with that of the respective absorber inserts. Of these, Boraflex_Fe had the highest $\% \Delta k / k_{ref}$ of 16.6906, followed by boraflex_Si with $\% \Delta k / k_{ref}$ of 16.635, with Alcan_SiB₄C14 having the lowest $\% \Delta k / k_{ref}$ of 13.5676.
- the second largest decrease was obtained when the absorber insert was placed outside the borated steel basket, as shown in Figure 3. This resulted in a decrease in k_{eff} ranging

between 9.3355% and 11.5914%. Again, Boraflex had the highest decrease followed by AA1100_Fe ($\% \Delta k/k_{ref} = 10.081$) and lastly ALCANfeB4C15 ($\% \Delta k/k_{ref} = 9.335$)

- the lowest decrease in k_{eff} (with the decrease ranging between 7.3231% and 8.4434%) was obtained when the neutron absorber was placed in the innermost region of the basket with the air gap surrounding it and then the borated steel on the outside (see Figure 2).

With regard to the end-effect design it was noted that the highest decrease (ranging from 5.409% to 6.0622%) was obtained when region 4 was made up of borated steel (in comparison to when the same region is made up of water). When water is used, the k_{eff} increases instead of decreasing, resulting in a negative $\Delta k/k_{ref}$.

In the central instrumentation tube design, 80% of the results indicated that the cord design would result in a much better decrease in k_{eff} , with $\% \Delta k/k_{ref}$ ranging from 0.27 to 2.025%, whereas in the sandwich design the $\% \Delta k/k_{ref}$ was found to range between 0.188% and 0.55%.

5.0 Analysis

Using the same design, all the absorber insert compositions result in a statistically similar change in k_{eff} , which (with the exception of ALCAN and its derivatives) may be explained by the fact that they all are made up of the same chemical elements which differ by a fraction of a percentage from one another.

When analysis was performed with the composition of borated steel replaced with any of the new absorber inserts, it was observed that the decrease in the k_{eff} depended largely on what the existing fuel assembly basket is made of. If the fuel assemblies are not shielded by any shielding material, as in the case where no re-racking has been done, placing them in the basket made up of the absorber insert material referred to above will result in a significant decrease in k_{eff} . If, however, there is already a basket in the spent fuel pool where the fuel assembly is located and it is made up of material which does not meet the characteristics of a good moderator, then changing the composition to that of the absorber insert cited above may be necessary.

The second best practically possible option would be to put a thin layer of the absorber insert inside or outside the existing fuel assembly basket. The results showed that if a 0.11 cm insert is placed on the outside of the existing basket an average $\% \Delta k/k_{ref}$ of 13.346 is obtained, which is significantly higher than when it is placed inside.

To understand why there is a difference in k_{eff} when the neutron absorber is inside compared to when it is outside the fuel assembly, it is important that the nuclear reactions that occur inside the global unit of the fuel assembly are examined and it is established which one of them is affected the most by the inclusion of the absorber inserts.

Since the purpose of the neutron absorber insert is to reduce the number of thermal neutrons interacting with the fuel, and given that most nuclear reactions indicated above take place inside the fuel cell, the first region of the global unit that the neutrons will interact with will determine what happens to those neutrons and what the final k_{eff} will be.

Table 2: Chemical composition of borated steel [4-6]

	Fraction in material composition	Macroscopic absorption cross-section (Σ_a)	Macroscopic scattering cross-section (Σ_s)	Logarithmic Energy of decrement (ξ)	Moderating ratio (MR)
Element	%	cm ⁻¹			
B	0.9	103	0.346	0.171	0.000574
Si	1	0.008	0.089	0.0698	0.776525
Mn	2	1.04	0.181	0.0359	0.006248
Cr	19	0.255	0.247	0.9872	0.956229
Fe	67.1	0.222	0.933	0.9881	4.152691
Ni	10	0.42	1.6	0.9887	3.766476
SUM					9.658743

Since a good moderator must have a large logarithmic energy decrement (ξ), a large scattering cross section (Σ_s) and a low absorption cross section, the materials found in the first region (innermost) of the global unit will be compared on the basis of their moderating ratio (MR), as given by Eq 2[10], in evaluating the effectiveness of the absorber material to reduce the k_{eff} .

$$MR = \frac{\xi \sum_s}{\sum_a} \quad \text{Eq 2}$$

Tables 2 and 3 show that the moderating ratios of the borated steel, the absorber inserts and water are 9.658743, 10.23803 and 71.17 respectively. This excludes the moderating ratio due to B₄C, since not all material contains B₄C. From this it is evident that the moderating ratio of the absorber insert is higher than that of borated steel. Since the higher the moderating ratio, the more effective the material performs as a moderator [10], this makes the absorber insert a much more effective moderator than borated steel, which also implies that borated steel is a much better neutron absorber than the other absorber inserts [10]. However, since for application as a neutron absorber insert and to be effective in that respect, the material must have a low moderating ratio, the borated steel would therefore be the best candidate of the three.

Table 3: Moderating ratio of materials used in the model [10]

	Σ_s	Σ_a	ξ	$\xi(\Sigma_s/\Sigma_a)$
	cm ⁻¹			
Al	0.08	0.02	0.07	0.40488
Si	0.09	0.01	0.07	0.776525
Fe	0.93	0.22	0.99	4.152691
Cu	0.61	0.03	0.03	0.579138
Mn	0.18	1.04	0.04	0.006248
Zn	0.24	0.07	0.03	0.100067
Mg	0.16	0.00	0.08	4.190167
Ti	0.23	0.33	0.04	0.028319
SUM				10.23803
B ₄ C	1.664	81.00	0.397	0.008156
H ₂ O	1.47	0.019	0.92	71.17

Therefore, to obtain the maximum benefit from the absorber insert, the borated steel must be on the inside and the proposed new absorber inserts on the outside. That is why the k_{eff} in Appendix 1 is lower when the neutron absorber is outside compared to when it is inside.

When an analysis is performed on the end-effect design, it is important that one takes into consideration the material inside region 4, which in the one case is water and in the other case is borated steel. In the case where region 4 is water, the k_{eff} is higher than that of the reference case, which has a k_{eff} of 0.719 and results in a negative $\% \Delta k/k_{ref}$. If, however, region 4 is borated steel, there is a decrease in k_{eff} resulting in a k_{eff} to the order of 0.6. The difference in k_{eff} between the reference standard and when region 4 is water can be explained by looking at unit 4 of the latter, where it is noted that it has an additional region, region 7, as the global region containing water, which the reference case does not have because the model does not need it. As a result of the extra amount of water contained in region 7 and the fact that the moderating ratio of water is high, i.e. 71.71, it results in an increase in k_{eff} and subsequently in the negative $\% \Delta k/k_{ref}$.

In this study two derivatives of ALCAN were developed, each containing 15.3% and 15.9% B_4C and referred to as ALCANfe B_4C_{14} and ALCANfe B_4C_{15} respectively. The results indicated that the presence of B_4C in ALCAN results in an increase in k_{eff} relative to that of their ALCAN parent which does not have B_4C . This is due to spectral hardening caused by the absorption of the thermal neutrons by B_4C , which would otherwise have reacted with ^{235}U and caused fission. As a result, there is an increase in the production of fissile isotopes of plutonium (i.e. ^{239}Pu and ^{241}Pu) from neutron capture by ^{238}U , which subsequently results in the fission from ^{239}Pu and ^{241}Pu exceeding that of ^{235}U . Consequently, there is an increase in k_{eff} where the B_4C neutron absorber is exposed to fuel assembly [11], as is the case in the basket design.

However, as shown in Appendix 1, this result depends on the design of the absorber insert and its material composition, as some designs tend to increase the k_{eff} whereas others will tend to decrease it. The increase in k_{eff} of ALCANfe B_4C_{14} and ALCANfe B_4C_{15} compared that of ALCAN_fe in the basket design is a good example of the contribution of ^{239}Pu and ^{241}Pu in fission, where the composition of the insert was such that conditions favoured the production of ^{239}Pu and ^{241}Pu . A similar case where in one design the k_{eff} will increase whereas another slightly different design will result in a decrease in k_{eff} can be found by comparing the k_{eff} of the design where in one case the neutron absorber insert is inside the borated plate basket and in the other case the neutron absorber is outside the borated plate basket. The results show that there is a decrease in k_{eff} in the former with an increase in B_4C , whereas in the latter case the k_{eff} increases with an increase in B_4C .

For the central instrumentation tube design, it was noted that 80% of the results indicated that when the neutron absorber is inserted in the instrumentation tube without a cladding the k_{eff} will be lower compared to when it has a cladding. The remaining 20% are split, with 10% showing that the k_{eff} will be the same whether it has a cladding or not, and the last 10% shows that without a cladding the k_{eff} will be marginally higher. This again may be ascribed to the amount of material exposed to neutron flux.

6.0 Conclusion

In conclusion, it has been established that the most effective design of all is the basket design made out of Boraflex. The $\% \Delta k/k_{ref}$ has been found to range between 7.32% and 16.69%, depending on the location of the Boraflex in relation to borated steel basket. The second most effective design has been found to be the end-effect design and, lastly, the central instrumentation design.

With regard to comparisons of effectiveness on the basis of material composition, it has been found that not only is ALCAN the least effective, but also that the inclusion of B_4C in its composition can have a negative effect, increasing the k_{eff} instead of decreasing it.

It is therefore essential that care is exercised when selecting both the composition of the aluminium composite materials and the design of the neutron absorber, as an incorrect selection may result in an increase in k_{eff} instead of decreasing it. This may, in turn, result in the unintended consequence of having to separate fuel assemblies even further to reduce the k_{eff} .

Appendix 1: Comparison of k_{eff} decrement obtained by application of various neutron absorber insets

	BASKET									END-EFFECT						CENTRAL INSTRUMENTATION TUBE					
	BASKET COMPOSITION CHANGED			INSIDE THE BASKET			OUTSIDE THE BASKET			Region4:H ₂ O			Region4:Borated Steel			SANDWICH			PIN/CORD DESIGN		
	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %	k_{eff}	σ	$(\Delta k/k_{ref})$ %
BORAFLEX_fe	0.599	0.001	16.691	0.663	0.001	7.710	0.635	0.001	11.591	0.725	0.001	-0.842	0.675	0.001	6.062	0.717	0.001	0.241	0.715	0.001	0.482
BORAFLEX_Si	0.599	0.001	16.635	0.667	0.001	7.157	0.637	0.001	11.362	0.726	0.001	-0.967	0.677	0.001	5.755	0.717	0.001	0.149	0.716	0.001	0.399
AA1100_fe	0.643	0.001	10.491	0.664	0.001	7.544	0.646	0.001	10.081	0.725	0.001	-0.912	0.676	0.001	5.984	0.714	0.001	0.572	0.715	0.001	0.505
AA1100_Si	0.616	0.001	14.319	0.666	0.001	7.331	0.646	0.001	10.165	0.724	0.001	-0.814	0.676	0.001	5.927	0.716	0.001	0.306	0.715	0.001	0.504
ALCAN_Fe	0.616	0.001	14.272	0.666	0.001	7.350	0.648	0.001	9.756	0.726	0.001	-1.023	0.674	0.001	6.265	0.715	0.001	0.437	0.715	0.001	0.427
ALCANfeB4C14	0.619	0.001	13.853	0.659	0.001	8.268	0.651	0.001	9.335	0.726	0.001	-1.001	0.678	0.001	5.702	0.715	0.001	0.561	0.701	0.001	2.409
ALCANfeB4C15	0.620	0.001	13.742	0.658	0.001	8.443	0.649	0.001	9.697	0.726	0.001	-1.027	0.677	0.001	5.734	0.716	0.001	0.292	0.701	0.001	2.451
ALCAN_Si	0.616	0.001	14.294	0.666	0.001	7.323	0.646	0.001	10.035	0.725	0.001	-0.870	0.676	0.001	5.912	0.716	0.001	0.344	0.715	0.001	0.447
ALCAN_SiB4C14	0.621	0.001	13.568	0.658	0.001	8.389	0.650	0.001	9.516	0.726	0.001	-0.985	0.679	0.001	5.535	0.716	0.001	0.316	0.702	0.001	2.367
ALCAN_SiB4C15	0.618	0.001	13.970	0.660	0.001	8.161	0.650	0.001	9.532	0.727	0.001	-1.130	0.680	0.001	5.410	0.714	0.001	0.636	0.702	0.001	2.246
Bounding (H₂O) Ref std	0.719	0.001																			

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