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# ACCELERATOR-DRIVEN-SYSTEMS TH-ADS BENCHMARK CALCULATIONS

## Results of Stage 1

W.E. FREUDENREICH H. GRUPPELAAR A. HOGENBIRK A.J. KONING

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#### Abstract

This report contains the results of calculations made at ECN-Petten of a benchmark defined to intercompare computational tools to calculate the reactor physics characteristics of Accelerator-Driven Systems (ADS). The benchmark exercise is made in the framework of an IAEA co-ordinated research programme. A simplified description of the Fast Energy Amplifier (FEA) restricted to the reactor part has been analyzed. All spectrum calculations have been performed with the Monte-Carlo code MCNP-4A and the JEF-2.2 nuclear data library. The following quantities have been calculated for three values of the effective multiplication factor for begin of life (BOL): <sup>233</sup>U-enrichments, source strength, source multiplication factor, void reactivity effect, radial and axial power distributions and radial spectral index distributions. Also some results of burnup calculations, performed with ORIGEN-S and FISPACT, are presented. A large spread in the evolution of  $k_{aff}$  is found due to different fission yields used in these calculations.

#### Acknowledgements

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### 1. INTRODUCTION

In the framework of their Co-ordinated Research Programme (CRP) on Accelerator-Driven Systems (ADS), the IAEA initiated an international calculational neutronics benchmark of an ADS with <sup>233</sup>U-<sup>232</sup>Th fuel. The simplified ADS specified for the benchmark is strongly related to the Fast Energy Amplifier (FEA) described in [1].

Goal of stage 1 of the benchmark is to study a number of reactivity effects as well as the reactivity burnup swing for different subcriticality levels of the system. The system is driven by an external spallation type neutron source. The spatial and energetic neutron source distribution is specified in the benchmark.

In an earlier report [2] results were given of the static calculations for begin-of-life (BOL) conditions performed with MCNP-4A [3] and, as far as possible, nuclear data based on the JEF-2.2 evaluation [4]. Because of a bug in MCNP-4A (see [2] and appendix A in this report) the nuclear data of the ENDF/B-VI evaluation (distributed with MCNP-4A) had to be used for <sup>233</sup>U. Report [2], containing the results, has been presented at a meeting in March 97 at Bologna (Italy). At this meeting also a number of additional requirements have been formulated to complete the first phase of the benchmark.

Meanwhile, the above-mentioned bug in MCNP-4A has been fixed at ECN. In this report the results of the recalculations for begin-of-life (BOL) conditions performed with MCNP-4A and using all nuclear data from the JEF-2.2 evaluation are presented.

In this report also results are presented of the burnup calculations for the benchmark. This calculations have been performed with our OCTOPUS [5] burnup and criticality code system. This system links the spectrum codes from the SCALE4.1, WIMS7 or MCNP-4A packages to the ORIGEN-S or FISPACT4.2 fuel depletion and activation codes.

### 2. BENCHMARK SPECIFICATION

A graphical representation of the ADS-geometry as modelled in MCNP-4A is given in figure 1. The system is cylinder symmetric around the vertical axis and symmetric around the midplane. The geometry is modelled exactly as specified in the benchmark description, see Appendix C. The radial and axial subdivisions shown in figure 1 were made to facilitate the calculation of power density profiles.



Figure 1 ADS-geometry (MCNP-4A model) with indication of material regions.

The nuclide densities at begin-of-life (BOL) for the regions 1 to 5, indicated in figure 1, are given in table 1. The materials in regions 1, 2 and 3 (fuel region) are at a temperature of 1200 K. The other materials, regions 4 and 5, are at a temperature of 900 K.

Nuclide	Region 1	Region 2	Region 3	Region 4	Region 5
<sup>232</sup> Th	_	-	7.45E-03	-	-
$^{233}\text{U} + ^{232}\text{Th}$	6.35E-03	7.45E-03		-	-
0	1.27E-02	1.49E-02	1.49E-02		-
Fe	8.10E-03	8.87E-03	8.87E-03	-	6.63E-03
Cr	1.12E-03	1.06E-03	1.06E-03	-	8.00E-04
Mn	4.60E-05	5.10E-05	5.10E-05	-	3.80E-05
W	4.60E-05	5.10E-05	5.10E-05		3.80E-05
Pb	1.77E-02	1.56E-02	1.56E-02	3.05E-02	2.41E-02
Total	4.6062E-02	4.7982E-02	4.7982E-02	3.05E-02	3.1606E-02

Table 1 Nuclide densities [(barn cm)<sup>-1</sup>] at BOL

Table 2 Spallation neutron spectrum (normalised to 1.0).

Upper energy boundary [MeV]	Source value
19.64	0.1985
4.99	0.152
3.03	0.178
1.84	0.165
1.11	0.122
0.675	8.0E-02
0.410	5.0E-02
0.248	5.45E-02
0.151	0

The neutron source region is located in a cylinder ( $\emptyset = 20$  cm, H = -25 to +25 cm) around the centre of the ADS. The material in this region is identical to that of region 4. The spectrum of the spallation neutrons produced in the source region is given in table 2. The quantities to be calculated for begin-of-life conditions are:

- $^{233}$ U enrichment for  $k_{eff} = 0.94$ ,  $k_{eff} = 0.96$  and  $k_{eff} = 0.98$ ;
- source strength of the external neutron source for the three values of k<sub>eff</sub> and a required thermal power of 1500 MW;
- void reactivity effects;
- radial and axial power distributions;
- radial spectral index.

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### 3. MCNP-MODEL

The Monte Carlo neutron transport code MCNP-4A has been used for all calculations for BOL conditions. The geometrical model is shown in figure 1 and the materials are listed in table 1. The nuclear data for all materials (nuclides) listed in table 1 were taken from JEF-2.2 and processed with NJOY-91.118 (with a number of ECN-updates). Materials 1, 2 and 3 were processed for 1200 K; materials 4 and 5 were processed for 900 K [4]. No self-shielding treatment has been applied to the unresolved resonance range. Continuous energy data have been used for all calculations.

Two different types of calculations were performed with MCNP-4A:

- KCODE calculations to determine k<sub>eff</sub> of the system (determination of the <sup>233</sup>Uenrichment and the void reactivity effects);
- fixed-source calculations (determination of the source strength necessary to produce 1500 MW fission power, the source multiplication factor k<sub>s</sub>, the source multiplication M<sub>s</sub>, the radial and axial power distributions and the radial spectral index).

The fixed source is located in a cylinder around the centre of the system (R = 10 cm) and its volume averaged spectrum is listed in table 2. Isotropic emission of the neutrons has been assumed.

#### 4. RESULTS AT BOL

### 4.1 <sup>233</sup>U-enrichment

As can be seen from table 1 the ADS-fuel (regions 1 and 2) is only specified by the summed density of  $^{233}$ U and  $^{232}$ Th. Open parameter is the enrichment of  $^{233}$ U in  $^{232}$ Th. The enrichment of  $^{233}$ U is defined by:

Enrichment( $^{233}$ U) =  $^{233}$ U density / ( $^{233}$ U +  $^{232}$ Th density).

The enrichment is the same for the fuel regions 1 and 2. For the benchmark the enrichment has to be determined for three different values of  $k_{eff}$  at BOL: 0.98, 0.96 and 0.94.

For a number of <sup>233</sup>U-enrichments  $k_{eff}$  calculations with MCNP-4A (KCODE option) were performed. The  $k_{eff}$ -values obtained from these calculations have been plotted in figure 2. This figure also shows a linear fit through the calculated points.

The <sup>233</sup>U-enrichments for the given values of  $k_{eff}$  at BOL are determined from the linear fit shown in figure 2 and are given in table 3. From figure 2 we also find that  $k_{eff}$  varies with about 0.006 per 0.1% variation of the <sup>233</sup>U-enrichment.



Figure 2  $k_{eff}$  at BOL as function of the <sup>233</sup>U-enrichment</sup>

Table 3<sup>233</sup>U-enrichment values for three given values for  $k_{eff}$  at BOL.

k <sub>eff</sub> (BOL)	Enrichment( <sup>233</sup> U)
0.94000	9.49 %
0.96000	9.81 %
0.98000	10.13 %

#### 4.2 Source strength

During its whole life the ADS has to stay in a subcritical state. To produce the required power of 1500  $MW_{th}$  the system has to be driven by an external neutron source. The power of the system can be adjusted with the source strength of the spallation type neutron source.

Using MCNP-4A in the fixed source mode with the neutron spectrum given in table 2 the fission energy released per source neutron was calculated. With this value the source strength necessary for a given power can be determined. The source strength depends also on the <sup>233</sup>U-enrichment which is characterized by the value of the effective multiplication factor  $k_{eff}$ . In table 4 the source strengths necessary for 1500 MW<sub>th</sub> (only energy released by fission is accounted for) are listed for the three given values of  $k_{eff}$  at BOL (these  $k_{eff}$ -values correspond to the <sup>233</sup>U-enrichment given in table 3). The fission Q-values of <sup>232</sup>Th and <sup>233</sup>U used in MCNP-4A are 171.91 MeV and 180.84 MeV, respectively.

The number of fission neutrons  $(F_s)$  produced from one external source neutron is given by:

$$F_{s} = (k_{1} + k_{1} \cdot k_{2} + k_{1} \cdot k_{2} \cdot k_{3} + ...) = (1 + k_{1} + k_{1} \cdot k_{2} + k_{1} \cdot k_{2} \cdot k_{3} + ...) - 1$$
  
=1/(1 - k<sub>s</sub>) - 1 = M<sub>s</sub> - 1

with the source multiplication  $M_s$  and the source multiplication factor  $k_s$ . The number of fission neutrons ( $F_s$ ) produced from one external source neutron is given in the output of a MCNP fixed source calculation were it is called the weight of fission neutrons created per source neutron. One then gets:

 $M_s = F_s + 1$  and  $k_s = (M_s - 1)/M_s = F_s/(F_s + 1)$ 

The values of  $M_s$  and  $k_s$  are also given in table 4.

<u>Remark</u>: The source multiplication  $M_s$  given here is different from the net multiplication M given before, in [2]. The net multiplication M is given in the output of MCNP and represents the net number of neutrons produced by a source neutron. This net number of neutrons is defined as the number of neutrons produced by fission- and (n,xn)-reactions minus the number of neutrons that are lost to these reactions. Because in [2]  $k_s$  had been calculated erroneously from M, the value of  $k_s$  from [2] is also different from  $k_s$  given here. The present approach should give the correct  $k_s$  value.

To characterise the average importance of spallation neutrons (external source) with respect to the internal sources the quantity  $\phi^*$  has been introduced.  $\phi^*$  is also called the effectiveness of spallation neutrons. The definition of  $\phi^*$  used here is somewhat different from that given in equation 8 of [6]). The definition used here (see [7] and appendix B) comprises a more consistent representation of the average importance of the internal fission source. The values of  $\phi^*$  are also given in table 4.

k <sub>eff</sub> (BOL)	S [n/s]	Ms	ks	φ*
0.9412	5.92·10 <sup>18</sup>	23.0 ± 0.4	0.9566 (7)	1.37 (3)
0.9603	3.82·10 <sup>18</sup>	35.1 ± 0.6	0.9715 (5)	1.41 (3)
0.9816	1.84·10 <sup>18</sup>	71.7 ± 1.8	0.9861 (4)	1.33 (5)

Table 4 Spallation neutron source strength S (needed for 1500 MW<sub>th</sub>), source multiplication  $M_s$ , source multiplication factor  $k_s$  and effectiveness of spallation neutrons  $\phi^*$  for three given values for  $k_{eff}$  at BOL.

#### 4.3 Void reactivity effect and fuel temperature effect

The ADS is cooled by liquid lead. In the case that the liquid lead runs away it is necessary that the system will stay in a subcritical state. In this benchmark only the void reactivity effect at BOL (defined by  $[k_{eff}(voided) - k_{eff}(BOL)] / k_{eff}(BOL)$ ) is required. For the three <sup>233</sup>U-enrichment values the void reactivity effect- and the  $k_{eff}$ -values at BOL for different voided regions are given in table 5. Negative values of the void reactivity effect are obtained for complete voiding of core regions 1 and 2.

Table 5 Void reactivity effect and  $k_{eff}$ -values for the three given  $k_{eff}$ -values (unvoided) at BOL for different voided regions.

	BOL (no void)	Region 1 voided	Regions 1 + 2 voided
k <sub>eff</sub>	0.94123 (44)*	0.94722 (47)	0.93385 (44)
[k <sub>eff</sub> (voided) - k <sub>eff</sub> (BOL)] / k <sub>eff</sub> (BOL)	-	0.0064±11%	-0.0078 ± 8.4%
k <sub>eff</sub>	0.96032 (48)	0.96811 (45)	0.95391 (45)
[keff(voided) - keff(BOL)] / keff(BOL)	-	0.0081 ± 8.4%	-0.0067 ± 10%
k <sub>eff</sub>	0.98155 (43)	0.98768 (47)	0.97241 (44)
[keff(voided) - keff(BOL)] / keff(BOL)	-	0.0062 ± 10%	-0.0093 ± 6.7%

\*): uncertainty in the last two digits.

In reactor safety analysis the fuel temperature coefficient of reactivity (FTC) is an important quantity. The FTC is defined by:

$$FTC = \frac{1}{k} \frac{\Delta k}{\Delta T}$$

Here the FTC is calculated only for the case of  $k_{eff}(BOL) = 0.96$  and a temperature change of the ThO<sub>2</sub> and UO<sub>2</sub> in regions 1, 2 and 3 has been considered. For this case the FTC becomes -4.6·10<sup>-6</sup> K<sup>-1</sup>.

### 4.4 Radial and axial power distribution

The thermal power (only fission) distributions were calculated in the MCNP-4A fixed source runs for the geometry subdivisions as shown in figure 1. The total fission power was set to 1500 MW<sub>th</sub>. Figure 3 shows the radial thermal power distribution (also listed in table 6) of the ADS in the centre plane ( $d = \pm 5$  cm) at BOL for the three systems. In particular for the lowest value of  $k_{eff}$  (0.94) the exponential behaviour is clearly visible.

Axial power density distributions were calculated for two different radial distances,  $r = 40\pm2.5$  cm (see table 7 and figure 4) and  $r = 145\pm2.5$  cm (see table 8 and figure 5).

radial	power density [W/cm <sup>3</sup> ]		
distance*	k <sub>eff</sub> = 0.94	k <sub>eff</sub> = 0.96	k <sub>eff</sub> = 0.98
35	518.9	441.1	353.5
40	456.8	392.9	324.4
45	410.3	358.9	306.2
50	372.7	332.5	289.5
55	341.2	311.2	276.3
60	313.3	291.1	265.2
65	288.6	273.0	254.2
70	265.8	255.7	244.3
75	246.3	239.9	232.8
80	226.7	225.3	222.3
85	244.5	246.6	247.0
90	226.6	229.4	233.7
95	209.0	214.6	220.9
100	190.1	198.0	206.8
105	173.9	182.5	192.4
110	158.2	167.9	177.7
115	143.0	151.5	162.4
120	127.4	136.5	146.7
125	112.7	121.5	131.6
130	99.7	107.1	116.5
135	86.8	93.8	102.5
140	75.1	80.9	89.0
145	65.7	70.6	78.3

Table 6 Average radial power density at centre plane (vertical average from -10 cm to +10 cm and radial average over rings with a radial thickness of 5 cm).

\*: mid radius of the radial rings.



Figure 3 Average radial power density at centre plane.

Table 7 Average axial power density from r = 37.5 to 42.5 cm (axial ring thickness = 10 cm).

axial	power density [W/cm <sup>3</sup> ]		
distance*	$k_{eff} = 0.94$	$k_{eff} = 0.96$	$k_{eff} = 0.98$
0	456.8	392.9	324.4
10	451.8	387.2	319.8
20	424.7	368.5	304.2
30	385.0	336.9	282.3
40	338.9	301.6	257.1
50	297.0	265.0	230.0
60	254.1	232.2	203.1
70	231.1	212.5	188.7

\*: axial mid of ring.

Table 8 Average axial power density from r = 142.5 to 147.5 cm (axial ring thickness = 10 cm).

axial	po	wer density [W/c	m³]
distance*	k <sub>eff</sub> = 0.94	k <sub>eff</sub> = 0.96	k <sub>eff</sub> = 0.98
0	65.7	70.6	78.3
10	64.8	69.6	78.0
20	62.9	67.9	75.6
30	59.7	64.9	72.1
40	56.3	60.9	68.1
50	52.2	56.3	62.8
60	48.4	53.0	57.8
70	51.9	55.0	60.5

\*: axial mid of ring.



Figure 4 Average axial power density at r = 40 cm



Figure 5 Average axial power density at r = 145 cm

#### 4.5 Radial spectral index distribution

For the characterisation of the neutron spectrum at BOL the radial dependence of the spectral index, SI, of above-threshold fissions in <sup>232</sup>Th and fissions in <sup>233</sup>U is asked for. This spectral index is defined by:

$$SI = \langle \sigma_f \rangle_{Th} / \langle \sigma_f \rangle_U$$

Here  $\langle \sigma_f \rangle_X$  stands for the spectrum averaged fission cross section of nuclide X. The fissionaveraged cross sections were calculated in the fixed source runs of MCNP-4A. Figure 6 shows a plot of the radial dependence of the fission spectral index SI for the three systems (see also table 9). The fastest (hardest) spectrum is seen in the spallation target region.



Figure 6 Average radial fission spectral index  $SI(^{232}Th/^{233}U)$  distribution.

radial	spectral ir	dex of fission SI(	<sup>232</sup> Th/ <sup>233</sup> U)
distance*	$k_{eff} = 0.94$	k <sub>eff</sub> = 0.96	k <sub>eff</sub> = 0.98
1.25	9.57E-03	8.28E-03	6.19E-03
5	8.64E-03	7.50E-03	5.54E-03
10	6.23E-03	5.38E-03	3.85E-03
15	3.22E-03	2.77E-03	1.97E-03
20	2.15E-03	1.88E-03	1.43E-03
25	1.70E-03	1.52E-03	1.31E-03
30	1.66E-03	1.61E-03	1.51E-03
35	2.13E-03	2.19E-03	2.17E-03
40	2.43E-03	2.50E-03	2.55E-03
45	2.55E-03	2.64E-03	2.69E-03
50	2.59E-03	2.71E-03	2.77E-03
55	2.63E-03	2.70E-03	2.79E-03
60	2.67E-03	2.71E-03	2.80E-03
65	2.69E-03	2.75E-03	2.83E-03
70	2.70E-03	2.79E-03	2.83E-03
75	2.71E-03	2.83E-03	2.85E-03
80	2.75E-03	2.84E-03	2.91E-03
85	2.86E-03	2.96E-03	3.02E-03
90	2.95E-03	3.00E-03	3.09E-03
95	2.94E-03	3.01E-03	3.13E-03
100	2.98E-03	3.06E-03	3.15E-03
105	3.05E-03	3.05E-03	3.15E-03
110	3.02E-03	3.02E-03	3.13E-03
115	3.03E-03	3.01E-03	3.15E-03
120	2.99E-03	3.02E-03	3.12E-03
125	2.93E-03	3.01E-03	3.12E-03
130	2.90E-03	3.01E-03	3.11E-03
135	2.88E-03	2.96E-03	3.0 <u>3E-</u> 03
140	2.73E-03	2.79E-03	2.87E-03
145	2.23E-03	2.34E-03	2.40E-03
150	1.15E-03	1.20E-03	1.21E-03
155	5.52E-04	5.89E-04	5.87E-04
160	2.68E-04	2.88E-04	2.83E-04

Table 9 Average spectral index of fission  $SI(^{232}Th)^{233}U$ ), vertical average from -10 cm to +10 cm.

\*: radial mid of ring.

### 5. RESULTS OF BURNUP CALCULATION

Burn-up calculations have been performed only for the case  $k_{eff}(BOL) = 0.96$ . As mentioned above our OCTOPUS [5] burnup code system has been used with MCNP-4A for the spectrum calculations. The burnup calculations have been performed for three burnup zones which are coincident with the three fuel zones defined in the benchmark.

For the burnup calculation both codes, ORIGEN-S and FISPACT, can be used. Within ORIGEN-S several reactor types may be chosen, which influences, within OCTOPUS, mainly the fission yield applied for the different fissionable isotopes. A number of different choices in the burnup codes have been tried to get an idea of their influence:

- 1. ORIGEN-S, LMFBR and constant flux within a burnup interval;
- 2. ORIGEN-S, LMFBR and constant power within a burnup interval;
- 3. ORIGEN-S, LWR and constant power within a burnup interval;
- 4. FISPACT and constant flux within a burnup interval.

In the cases 1 and 2 fast neutron fission yields are used for <sup>235</sup>U and <sup>238</sup>U. The yields for all other fissionable isotopes, including <sup>233</sup>U, are substituted by the fast fission yield of <sup>239</sup>Pu. This approximation is perhaps reasonable for <sup>238</sup>U/Pu fast reactors, but certainly not for <sup>233</sup>U/Th fast systems.

In case 3 thermal neutron fission yields are used for <sup>233</sup>U, <sup>235</sup>U and <sup>239</sup>Pu and fast fission yields are used for <sup>238</sup>U. The yields for all other fissionable isotopes are substituted by the thermal yield of <sup>239</sup>Pu.

In case 4 fission yields for 19 isotopes are available and the thermal and fast yield are weighted according to the actual neutron spectrum. From all four cases this is clearly the best method.

In all four cases the neuton spectrum has been calculated only once: at BOL. An additional exploring calculation showed that spectrum update during burnup has only a minor influence on  $k_{eff}$ . OCTOPUS uses the neutron spectrum to produce 1-group cross sections for all nuclides used explicitly in the spectrum calculation and for the remaining nuclides available in the multigroup ECNAF-library.

Figure 7 shows the evolution of  $k_{eff}$  with increasing burnup for the four cases mentioned above. The  $k_{eff}$ -values have been calculated with the KCODE option of MCNP-4A. In these calculations 52 fission products and 8 actinides have been used explicitly. No pseudos for fission products have been applied. It is estimated that the effect of missing fission products on the  $k_{eff}$  values is only marginal (< 0.002)

Figure 7 clearly shows that the constant flux or constant power option in ORIGEN-S does not influence the results. But the change from ORIGEN-S built-in LMFBR- to LWR-"yields" leads to much higher  $k_{eff}$ -values during burnup. The largest  $k_{eff}$ -values are obtained with FISPACT which uses the most realistic fission yields. Therefore, the upper curve in figure 7 represents the final ECN-result.



Figure 7 Evolution of  $k_{eff}$  with increasing burnup for four different code options. <u>The final</u> <u>ECN result is shown in the upper curve, calculated with FISPACT</u>.

### 6. COMPARISON OF RESULTS OBTAINED WITH LEAD DATA FROM JEF-2.2 AND EFF-2.4

The ADS-system described for this benchmark contains a large amount of lead. Therefore one may expect differences in the results dependent on the lead data used. The results presented in chapter 3 were obtained with data from JEF-2.2. As this ADS-system has a fast neutron spectrum we were interested in the results obtained with lead data, primarily evaluated for fusion applications: data from EFF-2.4. This data also have coupled energy-angular distributions for inelastic scattering and (n,2n)-reactions.

For the comparison we have chosen the case with  $k_{eff} = 0.96$ . The only difference between the calculations that are compared is the source of the nuclear data of lead. The first data set comes from the JEF-2.2 evaluation (used in this benchmark) and the second set comes from the EFF-2.4 evaluation.

The results for  $k_{eff}$  for the three cases, unvoided, region 1 voided and regions 1+2 voided, as well as the difference between the JEF-2.2 and the EFF-2.4 results are given in the table below.

BOL	regions 1+2 unvoided	region 1 voided	regions 1+2 voided
k <sub>eff</sub> (JEF-2.2)	0.96007 (40)	0.96876 (43)	0.95806 (45)
$k_{\rm eff}$ (EFF-2.4)	0.95573 (45)	0.96555 (42)	0.95511 (40)
[k <sub>eff</sub> (EFF) - k <sub>eff</sub> (JEF)]	-0.00434 (60)	-0.00321 (60)	-0.00295 (60)

For all three cases significant lower values for  $k_{eff}$  are obtained with the EFF-2.4 data. This result shows clearly the influence of the lead data used for this ADS-system.

#### Remark:

The calculation results, presented in this chapter (taken from [2]), were obtained with <sup>233</sup>U-data from the ENDF/B-VI evaluation.

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### 7. CONCLUSIONS

The strength and sign of the void effect is dependent on the voided region. Voiding of the central part (region 1) gives a positive void effect and voiding of regions 1 and 2 gives a negative void effect.

A negative fuel temperature effect of reactivity (FTC) has been found for the ADS.

In chapter 5 examples are given of the results for  $k_{eff}$  calculated with different lead data. The  $k_{eff}$ -values (for voided and unvoided cases) are significantly influenced by the choice of the nuclear data set for lead.

The evolution of  $k_{eff}$  in the burnup calculations shows a strong dependence from the fission yields used in these calculations.

Using ORIGEN-S for fast systems, fission yields of <sup>239</sup>Pu are used for <sup>233</sup>U. This may lead to erroneous results. It is recommended to modify ORIGEN-S such that fast fission yields of <sup>233</sup>U are used for fast system calculations containing <sup>233</sup>U in the fuel.

Finally, it is noted that the observed large spread in  $k_{eff}$  evolution between various participants may be due - at least partly - to the use of wrong fission yields for <sup>233</sup>U. This should be analysed in detail.

#### REFERENCES

- [1] Rubbia, C. et al., Conceptual design of a fast neutron operated high power energy amplifier, CERN/AT/95-44(ET), Geneva, Sept. 1995.
- [2] Freudenreich, W.E. and Hogenbirk, A., *Th-ADS Benchmark Calculations, Results of* Part I, ECN-Memo NUC-FYS--97-03, 71137/NUC/WF/mb/4817, February 1997.
- [3] Briesmeister, J.F.(Ed.), MCNP A General Monte Carlo N-Particle Transport Code, Version 4A, LA-12625-M, November 1993.
- [4] Hogenbirk, A., EJ2-MCNP, Contents of the JEF-2.2 based neutron cross section library for MCNP-4A, ECN-I--95-017, ECN-Petten, 1995.
- [5] Kloosterman, J.L., Kuijper, J.C. and de Leege, P.F.A., *The OCTOPUS burnup and criticality code system*, ECN-RX--96-032, June 1996.
- [6] Slessarev, I. and Tchistiakov, A., *IAEA ADS Benchmark (Stage 1), Results and Aanlysis*, Cadarache/DRN/CEA, presented at TCM-Meeting, Madrid, 17-19 September 1997.
- [7] Kruijf de, W.J.M. and Freudenreich, W.E., Validation of WIMS-7 for calculations on ADS, ECN-R--97-17, February 1998.

### APPENDIX A: MCNP-4A-BUG IN SAMPLING THE FISSION SPECTRUM

When we started with the calculations for this benchmark we got very bad results ( $^{233}$ Uenrichments of about 1.5% instead of about 10%). The reason was the treatment of the fission spectrum representation (LAW = 5) on the JEF-2.2 evaluation by MCNP-4A. The LAW = 5 representation is hardly ever used in nuclear data evaluations which might be the reason that this bug was not detected earlier.

For our first calculations for this benchmark, presented in [2], we therefore used <sup>233</sup>Udata from the ENDF/B-VI evaluation.

To illustrate the differences between JEF-2.2 and ENDF/B-VI data in combination with MCNP-4A we compare the neutron energy distribution sampled by MCNP-4A and the resulting neutron spectrum in the ADS-system.

The figure below shows the energy distribution of the neutrons sampled by MCNP from <sup>233</sup>U nuclear data of the JEF-2.2 and the ENDF/B-VI evaluations. A clear oversampling in the low energy range in the case of the JEF-2.2 data is observed.



The result of this difference in the sampled neutron energy is a completely different neutron spectrum of the ADS core as shown in the figure below.



### APPENDIX B: ON THE DEFINITION OF THE SPALLATION NEUTRON IMPORTANCE φ\*

Making use of the notation given in [6] and using the basic equations given there, from equation 1 of [6] it follows:

 $k_s / (1 - k_s) = \langle M\Phi \rangle / \langle S \rangle$ 

And from equation 3 of [6] it follows:

$$(1 - k_{eff}) / k_{eff} = \langle \Phi^*, S \rangle / \langle \Phi^*, M \Phi \rangle$$

Multiplying these equations gives:

$$\varphi^* = \frac{1 - k_{\text{eff}}}{k_{\text{eff}}} \frac{k_s}{1 - k_s} = \frac{\langle \Phi^*, S \rangle}{\langle S \rangle} \left( \frac{\langle \Phi^*, M\Phi \rangle}{\langle M\Phi \rangle} \right)^{-1}$$

with  $\frac{\langle \Phi^*, S \rangle}{\langle S \rangle}$  being the average importance of an external (spallation) neutron

and  $\frac{\langle \Phi^*, M\Phi \rangle}{\langle M\Phi \rangle}$  being the average importance of an internal (fission) neutron.

## APPENDIX C: ADS BENCHMARK DESCRIPTION

They have to be presented in the OUTPUT DATA. Table 1

Three values are proposed:  $K_{eff} = 0.98$ ; 0.96; 0.94

5.2. For every given  $K_{eff}$  (BOL) the evolution (function of time) curve has to be calculated :  $K_{eff} = f(t)$ , where  $t = 0 \div Error!$  Bookmark not defined. 2250 days, time step  $\Delta t = 150$  days of

continuous work. Simultaneously, a burnup scale (averaged over regions 1+2) (GWd/t of heavy atoms) has to be presented, which corresponds to the "time scale".

Note, that in every checkpoint (including BOL) an "eigenvalue" calculation of the  $K_{eff}$  value has to be produced, meanwhile, the neutron flux for "burnup" calculation has to be taken as a solution of diffusion equation with an external source. This source S (n/s) should be adjusted to maintain the given total power (1500 GWt).

All results have to be presented in the following form in OUTPUT DATA. Table 2.

**5.3**. Void reactivity effect (Table 3) :

Calculation of  $K_{eff}$  (BOL) for voided ADS-states:

1) Pb density is equal to 0 in region 1.

2) Pb densities are equal to 0 in regions 1+2

5.4. Spectral indices and power distributions :

Calculation of a radial  $\langle \sigma_f \rangle_{Th} / \langle \sigma_f \rangle_U$ - spectral indices distribution for BOL has to be presented on OUTPUT DATA. Fig. 1.

Calculation of a radial power distribution at BOL has to be presented on OUTPUT DATA. Fig 2.

**5.5**. Calculation of all inventory activities in Bq/g (cooling time :  $10^2$ ,  $10^3$ ,  $10^4$ ,  $10^5$ ,  $10^6$  years) at EOL (t = 2250 days) has to be presented in OUTPUT DATA. Table 4.

### Finally, one has the following OUTPUT DATA to present : Tables 1Error! Bookmark not defined.4 and Fig. 1,2.

### APPENDIX INPUT AND OUTPUT DATA

#### A1. INPUT DATA.

#### INPUT DATA. Table 1

Spallation neutron spectrum

Group number	Energy boundaries (MeV)	Source value
1	19.64 - 4.99	0.1985
2	4.99 - 3.03	0.152
. 3	3.03 - 1.84	0.178
4	1.84 - 1.11	0.165
5	1.11 - 0.675	0.122
6	0.675 - 0.410	8.0E-02
7	0.410 - 0.248	5.0E-02
8	0.248 - 0.151	5.45E-02
9	0.151 - 9.14E-02	0
10	9.14E-02 - 5.54E-02	0
11	5.54E-02 - 3.36E-02	0
12	3.36E-02 - 2.04E-02	0
13	2.04E-02 - 1.24E-02	0
14	1.24E-02 - 7.50E-03	0
15	7.50E-03 - 4.55E-03	0
16	4.55E-03 - 2.76E-03	0
17	2.76E-03 - 1.67E-03	0
18	1.67E-03 - 1.02E-03	0
19	1.02E-03 - 6.16E-04	0
20	6.16E-04 - 3.74E-04	0
21	3.74E-04 - 1.37E-04	0
22	1.37E-04 - 3.07E-05	0
23	3.07E-05 - 4.15E-06	0
24	4.15E-06 - 5.62E-07	0
25	5.62E-07	0

Nuclei	Region 1	Region 2	Region 3	Region 4	Region 5
<sup>232</sup> Th <sup>-</sup>			7.45E-03		
$^{233}\text{U}+^{232}\text{Th}$	6.35E-03	7.45E-03			
0	1.27E-02	1.49E-02	1.49E-02		
Fe,	8.10E-03	8.87E-03	8.87E-03		6.63E-03
Cr `	1.12E-03	1.06E-03	1.06E-03		8.00E-04
Мп	4.60E-05	5.10E-05	5.10E-05		3.80E-05
W	4.60E-05	5.10E-05	5.10E-05		3.80E-05
Pb	1.77E-02	1.56E-02	1.56E-02	3.05E-02	2.41E-02

INPUT DATA. Table 2 Nuclei densities (BOL) at 20°C.

A2. OUTPUT DATA.

s -	OUTPUT DATA. Table 1						
-	K <sub>eff</sub> (BOL)	Enrichment = ${}^{233}$ U density/( ${}^{233}$ U+ ${}^{232}$ Th density) in the regions 1 and 2 (BOL)					
	0.98						
	0.96						
	0.94						

### OUTPUT DATA Table 1

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#### OUTPUT DATA. Table 2

		$K_{eff} = f(t), \Delta t = 150 \text{ days}$										<u></u>				
BOL	В	150	300	450	600	750	900	1050	1200	1350	1500	1650	$1800$ $\rightarrow$ 100 GWd/t	1950	2100	2250
0.98	K <sub>eff</sub>															
0.96	K <sub>eff</sub>												- <u></u>			
0.94	K <sub>eff</sub>															

#### OUTPUT DATA. Table 3

	BOL (no void)	Region 1 voided	Region 1+2 voided
K <sub>eff</sub>			
$[K_{eff}(Voided) - K_{eff}(BOL)]/K_{eff}(BOL)$			

#### **OUTPUT DATA.** Table 4

Cooling time (years after irradiation)	10 <sup>2</sup>	10 <sup>3</sup>	104	105	10
Fuel Activity					

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