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Source Convergence Problems in the Application of Burnup Credit for WWER-440 Fuel

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The problems in Monte Carlo criticality calculations caused by the slow convergence of the fission source are examined on an example. A spent fuel storage cask designed for WWER-440 fuel used as a sample case. The influence of the main parameters of the calculations is investigated including the initial fission source. A possible strategy is proposed to overcome the difficulties associated by the slow source convergence. The advantage of the proposed strategy that it can be implemented using the standard MCNP features.

KEYWORDS: ***burnup credit, source convergence, WWER-440***

1. Introduction

The slow convergence of the source in Monte Carlo criticality calculations of loosely coupled systems is a widely known problem. Real-life examples of such systems occur in spent fuel storage. This effect has particular importance in the application of burnup credit, because an irradiated fuel assembly necessarily has higher burnup at its middle part and lower burnup at the ends. In the case of high burnup the reactive parts of the assembly are separated by the strongly absorbing central part. This may result slow or even erroneously identified source convergence which can lead to the underestimation of the multiplication factor.

The source convergence will be investigated on the example of a conceptual dual purpose cask designed for WWER-440 fuel. The axial length of such fuel is 244 cm, which is less then that of a typical PWR fuel. This may result less difficulties in source convergence. However, the regular use of absorber rods during normal WWER-440 reactor operation increases the asymmetry of the axial burnup distribution, which increases the source convergence difficulties according the recent experiences. The purpose of this paper is to develop a strategy which can help a criticality analyst in the identification of the properly converged k_{eff} and to get an estimation of the necessary number of neutrons and cycles.

2. A possible strategy for the investigation of the source convergence

In a Monte Carlo criticality calculation the basic factors influencing the accuracy of the calculations is the number of neutron per cycle, the number of cycles skipped and the number of active cycles. Using sufficiently large number of neutrons, the proper value of the k_{eff} can be calculated. However, the standard diagnostic features incorporated in Monte Carlo codes are not in every case sufficient to decide whether the convergence is achieved or not. The same holds for the fission distribution convergence.

It seems to be straightforward to use the role of the initial source in diagnosing the convergence. If we perform k_{eff} calculations with strongly different initial source, initially the calculated values of the multiplication factors will be different. When the fission fractions are apparently converged in the different calculations and the k_{eff} values resulting from calculations with different initial source are equal within the statistical error, it is reasonable to assume that the convergence is achieved.

According this strategy we suggest performing a series of calculations with different number of neutron per cycles, inactive and active cycles and with different initial sources. Beside, we define separate tallies for fission fraction in a number of layers and during the individual calculations periodically make complete printout for the tallies by the MCNP. (These periodic printouts will be referred as control steps.) Completing all the calculations

- Discard the cases when MCNP doesn't print final k_{eff} result because of normality check failure
- Discard the cases when MCNP give warning(s) for k_{eff}
- Check the periodic printout of the ten statistical checks for tallies. Discard the cases, when there is no at least a few control steps, when all the fission fraction tallies meet all the statistical checks
- Investigate the behavior of the statistical checks as function of control steps. Select those cases where all tallies meet all the checks during the last few control steps
- Investigate the fission fractions change in these control steps whether it is really so small as expected

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- Compare the fission fractions from those calculations which are seemed to be converged
- Compare the k_{eff} calculated from cases where the fission fractions converged inside a calculation and the fission fractions from different calculations are close to each other.

The advantage of this approach is that it can be implemented using the standard MCNP features. The feasibility of the method will be investigated on a sample case.

3. Investigation of the sample case

3.1 Description of the investigated system

The strategy described above was applied to a conceptual storage cask designed by using the burnup credit for WWER-440 fuel. The investigated case was taken from the CB4 burnup credit benchmark defined by Markova[1]. This benchmark is the last part of the burnup credit benchmark series which was studied in the AER collaboration of the WWER-440 reactor using countries and which corresponds to the burnup credit benchmark series organized by the OECD/NEA[2]. In the CB4 part of the benchmark series the influence of the axial burnup distribution on the criticality of a spent fuel cask was studied. In this benchmark a cask filled with 84 spent fuel assemblies was investigated. The horizontal cross section of the cask is shown on Fig. 1.

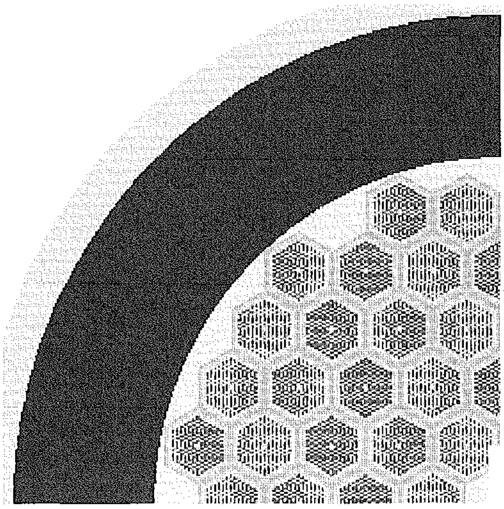

Fig.1 Horizontal cross section of the cask

The initial enrichment of the assemblies was 4.4 % and they had identical axial burnup distribution. In the case selected for examining the source convergence, the average burnup of the assemblies was 40 MWd/kgU and the cooling time was 5 years. 12 actinides and 15 fission products were considered in the calculations. The axial length of the active part of the fuel assemblies is 244 cm.

The assemblies were divided into ten axial nodes with equal length. The axial distribution of the burnup and the isotopic composition were given in these 10 nodes and were taken from the CB3+ WWER-400 burnup credit benchmark addition[3]. The detail of the geometry and material composition of the cask as well as of the fuel is given in the benchmark specification[1,3]. This problem has already been used for source convergence studies[4].

3.2 Description of the calculations

To examine the source convergence on a system with such characteristics, two sets of criticality calculations with different parameters were made for the cask. In the first set relatively small number of neutron was used: 5000, 10000 and 15000 neutron per generation, 50, 100 and 150 skipped and 800 active cycles were used. In the second set the corresponding numbers were 20000, 40000 and 60000 neutron per generation, 300, 500 and 700 skipped and 1000 active cycles. All calculated cases were investigated using four initial sources:

a, uniform source along the total axial length of the fuel

b, source in the nodes at the top

c, source in the nodes at the bottom

d, source in the nodes with highest burnup (third node from top). Loosely speaking this case will be referred as middle.

Altogether, both sets consist of 36 calculations. For the identification of the individual cases in a set the k/n/z abbreviation will be used. Here k is the number of neutron per generation in thousands, n is the number of skipped cycles in hundreds, and z refers to the initial source: U for uniform, T for top, B for bottom and M for highest burnup source. As an example, 15/0.5/T refers to a calculation with 15000 neutrons per generation, 50 cycles skipped and source is defined at the top.

The fission fraction was evaluated in ten layers corresponding to the nodes of the assemblies. The fission fraction in each layer was defined as a separate tally and they were printed after each 50 active cycles. The notation $F_{i,j}$ will be used for the fission fractions from a particular calculation. Here i is the number of the control steps and j is the number of the node.(The maximal value of i for the first set of parameters is 16, for the second set is 20.) The meeting of the ten statistical checks used by the MCNP is examined in these control steps. (It should keep in mind that as the result of a Monte Carlo calculation is subjected to statistical fluctuation, the same holds for the results of the statistical checks.)

In the following in comparison of two calculated values, y_1 and y_2 for example, their difference generally will be expressed as a relative quantity $\Delta = (y_1 - y_2)/\sigma_t$ where

$$\sigma_t = \sqrt{\left(\sigma_1^2 + \sigma_2^2\right)} \quad (1)$$

Here σ_1 and σ_2 are the variances of the two quantities to be compared. Loosely speaking the agreement is acceptable if Δ is less about two.

3.3 Results of the calculations using the first set of parameters

Using the first parameter set, in five cases MCNP even did not print final k_{eff} because of the total lack of normal distribution of the individual k_{eff} values. In these 5 cases the number of skipped cycles was 50 with bottom and middle initial source. Four other cases were discarded because MCNP issued some warning on k_{eff}.. In that cases also bottom and middle initial source was used with 50 or 100 skipped generation. Eight additional cases were excluded because there were no control steps when all tallies would have passed the 10 MCNP statistical tests. In these cases bottom, middle and uniform initial source was used with different combination of the two other varying parameters.

The closer look of the remaining seventeen cases shoes that the statistical tests shows quite random behavior during the calculations. This illustrated on the Table 1, where the number of tallies passed all MCNP statistical checks is sown as the function of the control steps for some sample cases. The total number of tallies is 10.

NC	5/0.5/T	15/0.5/T	5/1.5/M	10/1.5/U
1	7	6	7	4
2	7	10	7	8
3	10	9	8	6
4	8	10	6	9
5	10	9	6	10
6	10	10	10	10
7	10	9	9	10
8	10	10	10	9
9	10	10	10	8
10	10	10	10	10
11	7	10	8	8
12	10	10	8	9
13	10	10	9	8
14	10	10	8	7
15	10	10	8	8
16	10	10	8	8

Table 1 Number of tallies passed all statistical checks during the calculation for sample cases. NC is the number of control step.

From these seventeen cases there were six, where all the tallies passed all the MCNP statistical checks during the last four or more control steps. This choice of the last four control steps is somewhat arbitrary. These cases are as follows: 5/0.5/T, 5/1.5/U, 10/0.5/T, 10/1/T, 10/1.5/T and 15/0.5/T. These results are not quite similar which one can expect. An observable tendency is the good results with initial source at the top. Here it should be reminded, that the meeting of the statistical criteria is subjected to statistical fluctuation. There is no reason that the 15/0.5/T case would be superior to the 15/1/T or 15/1.5/T. Based on the statistical checks the case 15/0.5/T seems to be best: the statistical criteria were met during the last nine control steps. This case will be considered as reference case for this set of calculations.

For these best cases the "inner" convergence of the fission fraction distribution was examined during the last control steps. The change of the difference $F_{16,j} - F_{i,j}$ with varying value of i was considered for the different calculation. In several cases the difference was significantly higher than the supposed $\Delta \approx 2$. In some cases this difference was higher than two even in the last two control steps. This is illustrated on the example of 10/1/T shown on Table 2.

N	NC=12	NC=13	NC=14	NC=15
1	-2.81	-2.74	-2.47	-1.50
2	-3.63	-4.60	-2.60	-2.05
3	-5.14	-4.86	-2.74	-2.18
4	-6.09	-5.15	-3.61	-2.28
5	-5.07	-4.44	-3.44	-1.14
6	-1.65	-2.28	-2.28	-0.50
7	-0.53	-1.90	-2.33	-0.59
8	-0.27	-1.22	-0.61	0.39
9	1.60	2.48	2.10	0.66
10	2.75	3.84	2.99	1.13

Table 2 Deviation of the fission fractions from the finally calculated values for the last four control steps in the case of 10/1/T. N is the node number from bottom to top, NC is control step number. For these four control steps all MCNP checks were met for all of the nodes.

The source convergence seems to be even worse if we compare the final fission fraction distributions from different calculations with distribution from the reference case. This is shown in Table 3. for some sample cases. Examining the best six cases selected above, the differences frequently are as high as about Δ=10.

N	5/0.5/T	10/1/T	10/1.5/T	5/1.5/U
1	6.77	2.17	4.74	9.14
2	0.07	2.98	5.64	4.73
3	-8.45	4.73	7.68	6.70
4	-9.11	2.34	3.12	-1.69
5	-10.84	-3.95	-1.00	-7.12
6	-7.87	-5.21	-3.93	-9.09
7	-3.34	-5.14	-5.17	-5.25
8	-0.93	-6.68	-8.36	-4.25
9	3.24	3.66	2.99	2.73
10	4.77	7.67	7.86	7.20

Table 3 Difference among fission fractions calculated for different case compared to the reference case. N is the node number from bottom to top. For these cases all MCNP checks were met for all of the nodes during at least for the last four control steps.

This suggests that we reach quite poor source convergence, which is not very surprising because of the relatively low number of neutrons.

The reference value from the reference criticality calculation is k_{eff} = 0.85157 and σ = 1.9×10^{-4}. If we examine the five other cases qualified as "good" on the base of the MCNP statistical criteria, the maximal deviation from this reference case is Δ = 1.32, which is fairly good agreement. If the seventeen cases considered which were examined in details, the maximal deviation from this reference case is Δ= 2.58. The overall agreement between the multiplication factors is not bad, however, the large number of discarded cases shows that these parameters were not sufficient for that problem.

3.3 Results of the calculations using the second set of parameters

Using the parameters of the second set, there was only one case where MCNP gave warning on k_{eff}. This was the 20/3/M case which was discarded. No other cases had to be excluded because of the MCNP statistical checks, so 35 cases were considered.

Looking the statistical checks, a similar random behavior is found than in the previous calculations. This is illustrated on Table 4 for some sample cases.

NC	60/3/T	40/5/M	20/5/T	60/7/U
1	10	10	10	10
2	10	8	10	10
3	8	7	10	10
4	10	6	8	10
5	10	6	7	10
6	9	7	7	8
7	10	6	8	10
8	9	6	9	9
9	9	7	9	10
10	10	8	10	10
11	10	9	10	10
12	10	9	10	10
13	10	9	10	10
14	10	10	10	10
15	10	10	10	9
16	10	10	10	9
17	10	10	7	8
18	10	10	7	8
19	10	10	7	8
20	10	10	7	8

Table 4 Number of tallies passed all statistical checks during the calculation for sample cases. NC is the number of control step.

Somewhat surprisingly, now also six cases were found, where all the tallies passed all the MCNP statistical checks during the last four or more control steps. These cases are as follows: 20/5/B, 20/5/U, 20/7/M, 40/3/T, 40/5/M and 60/3/T. The tendency that the initial source at the top is effective is not present; however, the "best" case according the MCNP statistical checks is the 60/3/T. In its case all the statistical criteria are met during the last 11 control steps. Now this case is considered as reference case.

Examination of the "inner" convergence now shows much better picture than in the previous point. The change of the fission fraction during the last steps when all statistical criteria are met for all tallies is mostly less than 2. However, in some cases there are somewhat higher values of Δ than it is supposed. This is shown of Table 5. for the case of 60/3/T. Comparison of the final fission fractions from different calculations also shows significantly better picture, but in some cases still there are quite essential difference, as it is shown on Table 6.

N	NC=16	NC=17	NC=18	NC=19
1	2.72	2.96	0.89	-0.39
2	2.89	3.29	0.04	-0.85
3	2.72	3.10	0.73	0.31
4	3.30	3.05	0.25	0.01
5	1.77	1.92	-0.30	0.13
6	1.22	0.64	-0.23	0.10
7	2.08	1.05	0.21	-0.66
8	1.88	0.95	0.72	-0.29
9	-1.68	-1.49	-0.36	-0.03
10	-3.30	-2.30	-0.60	0.78

Table 5 Deviation of the fission fractions from the finally calculated values for the last four control steps in the case of 60/3/T. N is the node number from bottom to top, NC is control step number. For these four control steps all MCNP checks were met for all of the nodes.

N	20/5/U	20/7/M	40/3/T	40/5/M
1	4.88	10.22	-1.95	-1.70
2	8.44	8.92	0.16	0.15
3	5.34	7.81	-1.31	-0.77
4	-6.87	3.07	-4.20	-2.89
5	-2.78	3.63	-0.55	1.61
6	-5.29	-0.13	-8.11	-2.54
7	1.23	-1.58	-4.80	-2.05
8	-0.56	-1.96	-1.14	-5.29
9	0.54	-2.12	3.46	0.10
10	1.75	-0.29	4.31	6.55

Table 6 Difference among fission fractions calculated for different cases compared to the reference case. N is the node number from bottom to top. For these cases all MCNP checks were met for all of the nodes during at least for the last four control steps.

The reference value for the multiplication factor from the case 60/3/T is k_{eff} = 0.85138 and σ = 0.8×10^{-4}. Compared this value with cases qualified as "good" on the base of the MCNP statistical criteria, the maximal deviation from the reference case is Δ = 2.05. If we consider the thirty five cases which were examined in details, the maximal deviation from this reference case is Δ= 2.48.

The absolute value of the difference between the minimal and maximal values of k_{eff} for these 36 calculations is 5.8×10^{-4}. This spread seems rather small compared that 3 different numbers of neutron per generation, 3 different number of inactive cycles and 4 different initial sources were used. This probably can be explained by the large number of neutrons used in any combinations. This number was high enough that the k_{eff} values calculated by different initial source converge close to each other. This phenomenon is illustrated on Fig.2.

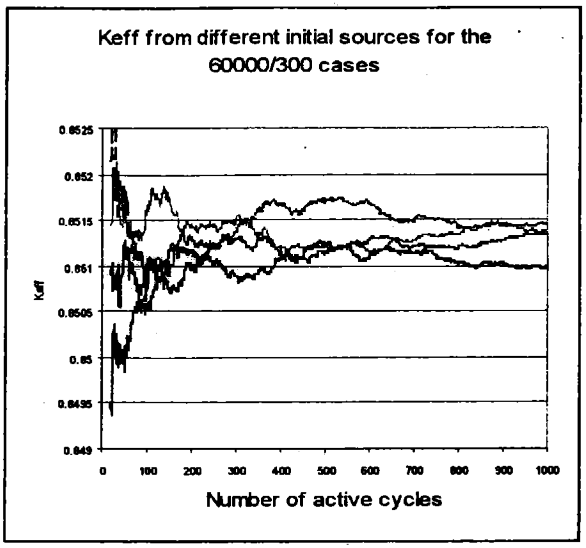

Fig. 2 K_{eff} calculated by four different initial sources as function of the active cycles.

On this figure the three upper curves corresponding to uniform, top and middle initial source come very close to each other. The curve due to the bottom source tends to a lower value. The difference to this lower value in k_{eff} is about 3.8×10^{-4}.

This small spread in keff suggests that the number of neutron used in the calculations is sufficient to calculate the multiplication factor with widely varying initial source. The question whether this small spread of the multiplication factor is true with lower number of active cycles but keeping the other parameters unchanged was examined. The difference of the maximal and minimal keff as the function of the number of active cycles was evaluated for the 36 combination of neutrons per generation, passive cycles and initial sources used in the previous calculations. The result is shown on Fig. 3.

It can be seen. that above 800 active cycles the spread is practically unchanged and above 600 the spread is still bellow about 10^{-3}. This suggests that the use of 700-900 active cycles is sufficient for such problems using similar set of the other parameters.

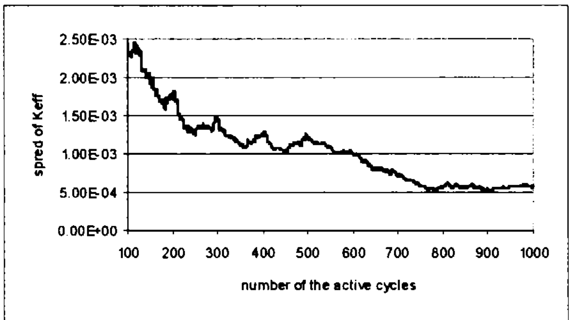

Fig. 3 Change of the k_{eff} spread with active cycle number

4. Conclusions

The convergence of the fission source was examined on the example of a WWER-440 spent fuel storage cask. For the investigations standard MCNP features were used only. The strong fluctuation of the number of passed statistical checks during the calculations was observed. Using different initial fission sources for diagnosing the convergence of the multiplication factor was found to be useful. The discrepancies in the fission source sometimes have only minor influence on the multiplication factor. It was found that for this type of criticality problems a few times ten thousand neutrons per generation, a few hundred skipped cycles and 600-700 or more active cycles is necessary.

Acknowledgements

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