A comparison of bounding approach with isotopic correction factors and Monte Carlo sampling in burnup credit method

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Abstract—**One of the methodologies used in criticality safety analysis is burnup credit method, which allows considering fuel burnup in models with spent fuel. This removes excessive conservatism from the analysis, but it also brings new uncertainties originating from computational prediction of spent fuel composition. The burnup credit method offer several possibilities of how to deal with this problem, e.g. using bounding approach with correction factors on nuclide concentrations, which is simple, but still very conservative approach. Another option is Monte Carlo sampling, which aims at receiving the most realistic result as possible, but is very computationally demanding. In this work, we have analyzed correction factors for selected nuclides and compared the results of both methods on model of spent fuel storage pool. The results show how much conservative the bounding approach is – in this case, the multiplication factor was higher by almost 0.03 than in Monte Carlo sampling, exceeding the standard deviation by more than 5.4 times.**

Keywords —**Bounding approach, Monte Carlo sampling, Burnup credit, SCALE**

I. INTRODUCTION

WHEN evaluating the nuclear safety of a system, a criticality analysis is performed in order to determine whether the system meets the requirements of the local regulations. The regulation requirements could be summarized in simplified form as:

$$k_{eff} + \sum \Delta_i \le k_{limit},$$

where k_{eff} is calculated value of effective multiplication factor of the evaluated model, which should be less than or equal to limit value k_{limit} (usually defined by legislation), if all biases and uncertainties marked as Δ_i are included.

Burnup credit is an approach that credits the reduction in reactivity due to fuel burnup. The calculation using burnup credit method consists of two main steps: a burnup calculation, which estimates nuclide concentrations in the spent fuel, and criticality calculation, which uses the nuclide concentrations determined in the first step. However, computational prediction of fuel composition introduces an additional source of bias or uncertainty. There are several methods that deal with these uncertainties and in general, they can be divided into two main categories: bounding methods and best-estimate methods.

The bounding approach aims to get the most conservative result by adjusting the concentrations of nuclides in a system. The concentration of selected nuclides in the model is multiplied by correction factors (referred to also as the isotopic correction factors) so that concentrations of fissile nuclides are increased and concentrations of absorbing nuclides are decreased. This leads to a more reactive system with the conservative estimate of multiplication factor k_{eff}.

The best-estimate methods aim to determine the uncertainty in spent fuel in a more accurate and realistic way. This can be done by using Monte Carlo sampling of the different parameters in a model based on their uncertainty and selected distribution. Other options, such as direct-difference method or sensitivity calculations, are also possible.

In this paper, we have tried to investigate how different the results of both methods are and what impact this could have on the possible compliance with regulatory limits.

II. CORRECTION FACTORS

Correction factors (CF) are part of validation of each calculation code. The factors are calculated from difference between the experiment and the calculation (E/C) based on PIE experiments results. The mean E/C value of a given nuclide is increased or decreased (depending whether it is fissile or absorbing nuclide) by the value of its standard deviation multiplied by the tolerance-limit factor.

The value of tolerance-limit factor is determined by the number of measured samples in PIE experiments. If more than 10 measurement data are available for a nuclide, a two-sided tolerance-limit factor is used at statistics with 95 % certainty and 68.3 % population. For fewer than 10 measurement data, one-sided tolerance-limit factor is used with 95 % certainty and 95 % population. In our case, the number of samples varied from 8 to 46, which is equivalent to tolerance factor of 3.14 (for 8 samples) to 1.22 (for 46 samples).

In this work, the correction factors were determined for a set of 40 nuclides based on PIE experiments [5] , [6] and [7] . The correction factors were analyzed for calculation codes from SCALE code system, the results are shown in Table I.

During this analysis, some modifications have been made. As the nuclide ^{103}Rh was not measured in PIE experiments, its correction factor was estimated to be the same as in the case of

[109]Ag, which is the closest fission product in terms of weight while also having low value of its correction factor. Another problem was caused by isotopes [151]Eu and [153]Eu, which were measured with high deviation and thus leading into negative value of their correcting factor. Their correction factor was therefore set to zero.

Additional analysis was also made for isotopes of gadolinium contained in pins with Gd_2O_3 burnable absorber, as these data are not part of PIE experiments. The Gd cross-sections were conservatively modified by their 3σ deviation from uncertainty library, the impact of modified cross-sections was then studied during burnup calculation and correction factors values were determined as a function of burnup, as can be seen in Fig. 2.

III. CALCULATION

The comparison of both methods was made on TVSA-T Gd-2M+ 4.76 fuel assemblies. In burnup calculation, a 2D model of the fuel assembly was used. The fuel pins were divided into 15 groups with respect to 30°symmetry. The isotopic composition of the fuel was then calculated by TRITON deterministic code from SCALE code system and ENDF/B-VII.1 library in 252-group broadened energy structure.

In criticality calculations, only 47 nuclides were considered in spent fuel composition – this includes 40 nuclides listed in Table I, 6 more isotopes of gadolinium and nuclide ^{16}O, which is part of UO_2 and Gd_2O_3 compounds. The calculations were made on simplified 3D model of spent fuel pool. It consists of lattice filled with fuel assemblies with same symmetry as in burnup calculation. Each assembly is inserted into boron steel hexagonal tube, as is pictured in Fig. 2. The lattice is placed on stainless steel support plate, under which is a layer of moderator and concrete with steel lining. The pool is flooded with clean water with density conservatively assumed as 1.0 g/cm^3.
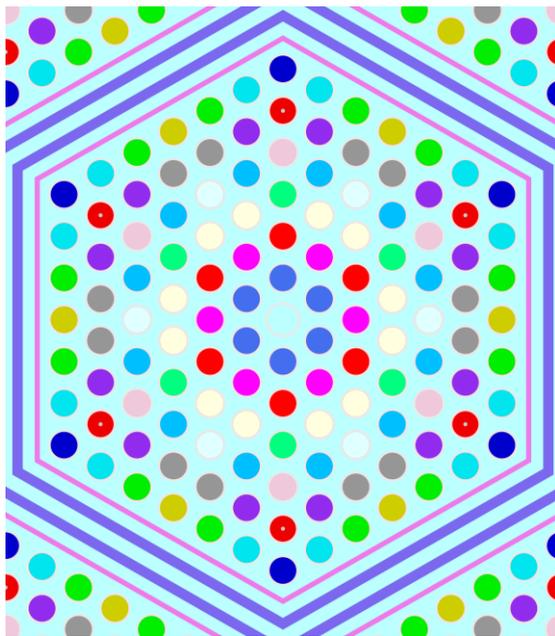

Fig. 1. Detail of fuel assembly in spent fuel pool calculation model.

TABLE I
CORRECTION FACTORS ANALYZED FROM PIE EXPERIMENTS

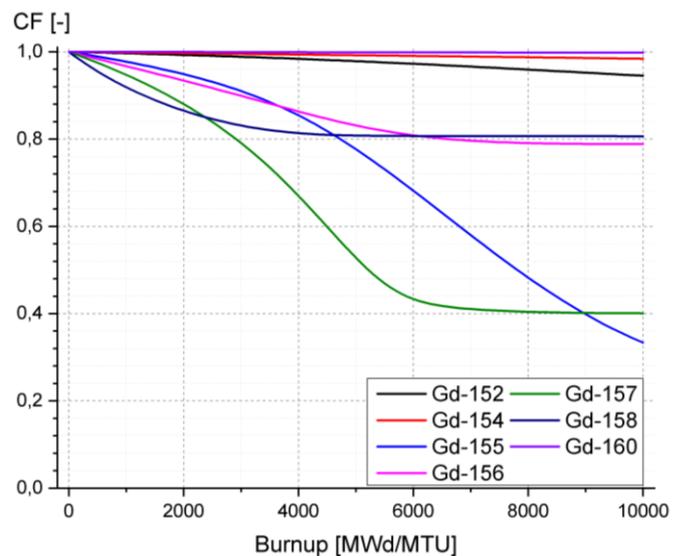| Nuclide	Mean E/C	Deviation E/C	CF	CF (used)
Mo-95	0.98	0.02	0.912	0.912
Tc-99	0.99	0.02	0.934	0.934
Ru-101	1.00	0.02	0.939	0.939
Rh-103	0.00	0.00	0.311	0.311
Ag-109	0.56	0.08	0.311	0.311
Cs-133	1.01	0.02	0.938	0.938
Cs-134	1.09	0.13	0.678	0.678
Cs-135	1.01	0.03	0.922	0.922
Cs-137	1.02	0.02	0.952	0.952
Ce-140	1.00	0.02	0.932	0.932
Ce-142	0.99	0.03	0.913	0.913
Nd-142	1.03	0.09	0.749	0.749
Nd-143	0.99	0.02	0.912	0.912
Nd-144	1.01	0.03	0.926	0.926
Nd-145	1.08	0.04	0.962	0.962
Nd-146	0.93	0.01	0.893	0.893
Nd-148	1.01	0.02	0.963	0.963
Nd-150	1.00	0.02	0.944	0.944
Sm-147	0.99	0.07	0.769	0.769
Sm-148	1.10	0.06	0.920	0.920
Sm-149	0.91	0.08	0.654	0.654
Sm-150	0.99	0.05	0.814	0.814
Sm-151	0.93	0.07	0.710	0.710
Sm-152	0.93	0.06	0.757	0.757
Sm-154	0.95	0.06	0.774	0.774
Eu-151	0.45	0.36	-0.666	0.000
Eu-153	0.18	0.06	-0.021	0.000
Gd-155	0.16	0.02	0.086	0.086
U-234	0.99	0.16	0.801	0.801
U-235	0.97	0.06	1.048	1.048
U-236	1.05	0.08	0.945	0.945
U-238	1.00	0.00	1.000	1.000
Np-237	1.47	0.59	0.627	0.627
Pu-238	1.20	0.26	0.879	0.879
Pu-239	0.97	0.10	1.089	1.089
Pu-240	1.00	0.07	0.906	0.906
Pu-241	1.02	0.11	1.158	1.158
Pu-242	1.06	0.22	0.787	0.787
Am-241	1.02	0.04	0.880	0.880
Am-243	0.87	0.18	0.654	0.654

Fig. 2. Correction factors for isotopes of gadolinium in pins with Gd_2O_3 burnable absorber as a function of burnup.

A. *Bounding Approach*

In bounding approach, the concentrations of nuclides were adjusted using correction factors CF mentioned above. The criticality calculation was then made for 21 steps of fuel burnup, calculated by KENO-VI code from SCALE system. The results are shown in Fig. 3. The maximum of effective multiplication factor is in this case at 8000 MWd/MTU, with a value of:

$$k_{eff} = 0.94309 \pm 0.00016.$$

As this is the highest achievable k_{eff} value, it is also a crucial point from the nuclear safety perspective and was therefore investigated further in case of Monte Carlo sampling.

B. *Monte Carlo Sampling*

In Monte Carlo sampling, the correction factors were not used. Instead, the concentrations of nuclides were multiplied by a factor from a set of pseudorandom numbers, which were generated with normal distribution based on E/C value and its standard deviation as shown in Table I. Each nuclide in each pin has therefore its own unique concentration, while also satisfying its probability distribution (see Fig. 5).

As the sampling method is more computationally demanding than the standard bounding approach described above, we have analyzed only the case with maximum multiplication factor, which is according to the previous calculation at burnup of 8000 MWd/MTU. A total of 5000 calculation cases were created, from which the first case was sampled in unperturbed state, where nuclide concentrations were multiplied only by mean E/C value and the deviations were not considered. All other cases are perturbed, i.e. they were sampled according to the procedure described above.

The samples were calculated in criticality calculation by transportation code KENO-VI from SCALE code system. The results are individual values of multiplication factor k_i of sampled cases i. The mean value $\bar{k}$, as well as corrected sample standard deviation s, of all perturbed cases was determined:

$$\bar{k} = \frac{1}{n}\sum_{i}^{n} k_i,$$

$$s = \sqrt{\frac{1}{n-1}\sum_{i}^{n}\left(k_i - \bar{k}\right)^2}.$$

This leads to a final result – the effective multiplication factor of all perturbed cases:

$$k_{eff} = 0.91374 \pm 0.00542,$$

which is close to multiplication factor of unperturbed case k_0:
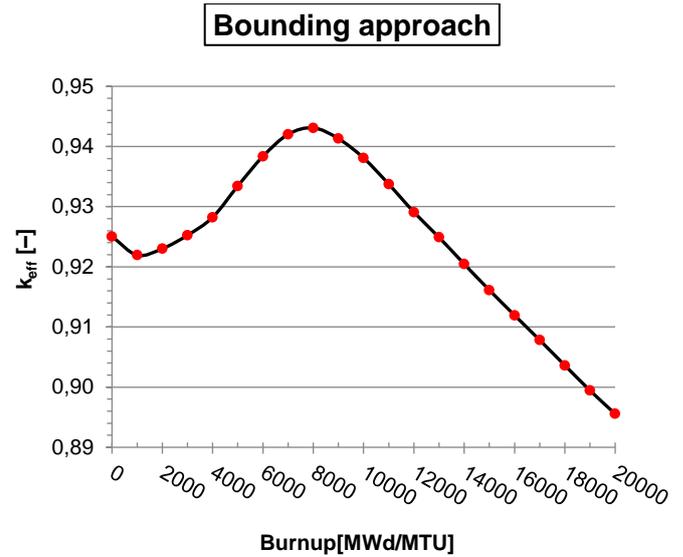
$$k_0 = 0.91872 \pm 0.00013.$$

Fig. 3. Multiplication factor based on fuel burnup calculated by bounding approach with correction factors on spent fuel pool model.
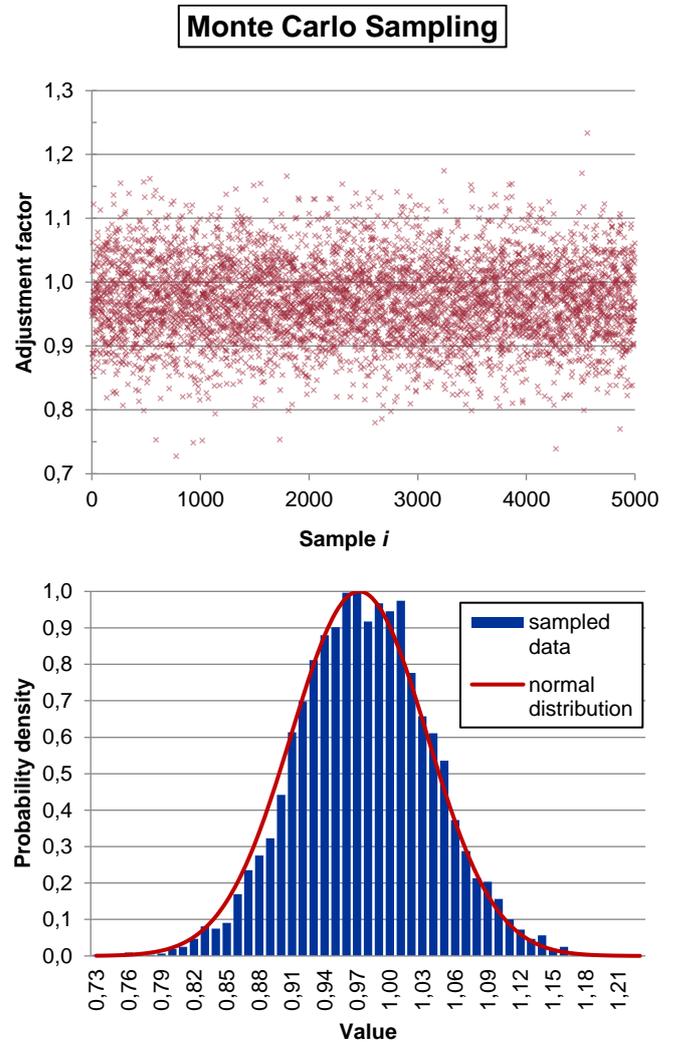

Fig. 4. Example of adjustment factor sampling for U-235 in one of the pins and its probability density function. In this case, the factor was sampled according to normal distribution with mean μ = 0.97 and deviation σ = 0.06.

IV. RESULTS

The results of both methods can be summarized as follows:

- Bounding approach:

$$k_{eff} \text{ (BA)} = 0.94309 \pm 0.00016.$$

- Monte Carlo sampling:

$$k_{eff} \text{ (MC)} = 0.91374 \pm 0.00542.$$

In this case, the multiplication factor calculated by bounding approach is higher by 0.02935, which is about 5.4× more than the value of the standard deviation of the sampled Monte Carlo tasks. The comparison shows how much conservative the bounding approach is.

The using of Monte Carlo sampling method can reduce the maximum multiplication factor for models where the coefficient is slightly above the legislative limit based on the current conservative burnup credit methodology. This could lead to an alleviation of possible restrictions resulting from the limit exceeding. However, it should be kept in mind that Monte Carlo sampling approach requires a calculation of large number of tasks and is therefore more computationally demanding.
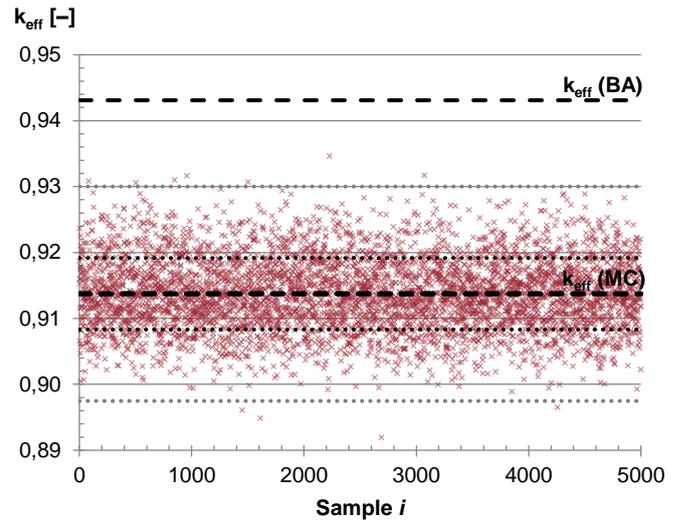

Fig. 5. Comparison of results calculated by bounding approach – k_{eff} (BA), and Monte Carlo sampling – k_{eff} (MC), with its standard deviation represented by dotted line. Results of individual samples k_i are also shown (represented by red crosses).

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