Sufficiency of Available MOX Experiments for Criticality Validation of VVER Burnup Credit Application

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Abstract

Applicability of the publicly available critical experiments for criticality code validation is investigated on the example of a compact storage pool containing VVER-440 fuel. New tools based on sensitivity/uncertainty method available in the SCALE6 program package are used. Similarity of the sample application and 234 critical experiments was investigated by means of c_k index calculated by the TSUNAMI-IP module of SCALE. In spite of the fairly good coverage of application sensitivity by the composite sensitivity of experiments, only modest degree of similarity was found (maximal c_k was slightly higher than 0.8). The application of extrapolation to $c_k=1$ is questionable in such cases, and it gives excessively limiting results. Because of the good coverage, the GLLSM method also was applied using the TSURFER module of scale. The calculated results seem reasonable, but the convergence of the procedure is doubtful.

Introduction

Use of computer codes for criticality safety evaluation requires the determination of the uncertainty of calculated multiplication factor due to error of nuclear cross sections. For this purpose, regulations generally prescribe the use of such critical experiments which are "similar" to examined application. Traditionally, the applicability of an experiment was based on physical characteristics, such as enrichment, H/U ratio, composition, energy of average group lethargy causing fission etc. Generally, trending analysis was performed against one of these variables, and the upper safety limit of k_{eff} including this uncertainty was determined by interpolation to the value of that variable characteristic to the investigated application. For burnup credit validation generally MOX experiments were used. The composition of fuel used in the publicly available MOX experiments is quite different from the composition of burned fuel, so selection of appropriate experiments based on traditional method is rather difficult. However, development of sensitivity/uncertainty methods and their incorporation into the modules of SCALE program package gives new tools for such investigations.

TSUNAMI-3D module evaluates the multiplication factor of the investigated system and its sensitivities to the group-wise cross sections of its constituent nuclides. The uncertainty of k_{eff} due to the error of nuclear data is determined by the formula $\sigma^2_X = \mathbf{S C S^T}$, where S is the sensitivity vector of k_{eff} and $\mathbf{C}$ is the covariance matrix of nuclear data and T denotes transposition.

Several important quantities are introduced in the TSUNAMI-IP module to quantify the similarity of different systems systems. At present, the most widely used is the similarity index c_k. If we have I systems having multiplication factors ki, i=1,..,N, we can define the relative sensitivity matrix S^k as $S^k_{ij} = \dfrac{\Sigma_j}{k_i}\dfrac{\partial k_i}{\partial \Sigma_j}$, where Σj is the group wise cross section of a specific of specific reaction of a specific nuclide. j=1,..,K, where K=number of nuclides x number of considered reactions x number of energy groups. Such set of system generally consists of one or more application (k_{eff} is not known from measurements) and several experiments (k_{eff} is known from measurements). If $\mathbf{C_{\alpha\alpha}}$ now denotes the relative covariance matrix, than the uncertainty matrix for the system k_{eff} values is given by $\mathbf{C_{kk}} = \mathbf{S_k C_{\alpha\alpha} S^T_k}$. If the c_{ij} similarity coefficient between the systems i and j is 1.0 it means full correlation, 0 means no correlation. If one of the systems is the investigated application, this index can be used as trending parameter in the statistical analysis of benchmark experiments and extrapolating its value to 1.0 the upper safety limit for the application can be derived. This procedure can be performed by the USLSTAT routine of SCALE.

Another important concepts introduced in TSUNAMI-IP is the completeness of coverage. The completeness parameter is defined by comparing the magnitude of each group-wise sensitivity coefficient for the application with respect to each of the corresponding sensitivities of the benchmark systems.

The TSURFER module is included into the latest version of SCALE. It is based on the generalized linear least square (GLLSM) method. In this method the discrepancies of the calculated and measured multiplication factors of experiments are reduced by adjusting the cross sections and experimental values so that the overall consistency is maximized. Uncertainties and correlations in nuclear data and critical experiments are taken into account in the process. Let us note the vector of measured multiplication factor is denoted by $\mathbf{m}$, the vector of calculated multiplication factor denoted by $\mathbf{k}$ and the vector of nuclear data denoted by $\mathbf{\alpha}$. The goal of GLLSM to find a transformation of nuclear data ($\alpha \rightarrow \alpha'$) and the measured multiplication factor ($\mathbf{m} \rightarrow \mathbf{m'}$) that they are most consistent with their uncertainty matrices. This is done by minimizing the following expression

$$\chi^2 = [\frac{\alpha'-\alpha}{\alpha}]^T C_{\alpha\alpha}^{-1}[\frac{\alpha'-\alpha}{\alpha}] + [\frac{m'-m}{m}]^T C_{mm}^{-1}[\frac{m'-m}{m}] ,$$

$$= [\Delta\alpha]^T C_{\alpha\alpha}^{-1}[\Delta\alpha] + [\Delta m]^T C_{mm}^{-1}[\Delta m]$$

where $\mathbf{C_{\alpha\alpha}}$ and $\mathbf{C_{mm}}$ is the uncertainty matrix of nuclear data and measurements, the elements of $\mathbf{\Delta\alpha}$ and $\mathbf{\Delta m}$ are the relative difference of the corresponding elements before and after the transformation. (Note that within the limitation of first order sensitivity theory $\mathbf{m'} = \mathbf{k'(\alpha')}$. Finding the transformation that results this minimum, the corrected multiplication factor of the application and its accuracy can be estimated.

Chi-square in the above expression is a quadratic form indicating the squared magnitude of the combined data variations with respect to their uncertainties. In the simple case when the uncertainty matrices are diagonal, it reduces to

$$\chi^2 \rightarrow \sum_{n=1}^{M} \left(\frac{\alpha_n' - \alpha_n}{\tilde{\sigma}_{\alpha_n}} \right)^2 + \sum_{i=1}^{I} \left(\frac{m_i' - m_i}{\tilde{\sigma}_{m_i}} \right)^2$$

TSURFER provides checks that a given set of benchmark experiments is consistent; that is, that the input responses have chi square value acceptably close to the estimated minimal value. The code progressively removes individual experiments until the calculated χ^2 is less than the target value specified in the input. Each iteration removes one experiment estimated to have the greatest impact on chi-square per degree of freedom. Details of the methods used to assess individual contributions is described in the SCALE manual [1].

As a sample application, a compact storage pool containing VVER-440 fuel with 4.4 % enrichment and 25 MWd/kgU burnup was investigated. Only the U-235, U-238, Pu-239, Pu-240, Pu-241 and O-16 content of the fuel were considered in the calculations. The pool was considered horizontally infinite, at top and bottom water reflector was taken into account. A horizontal cross section of this geometry model is shown on Fig.1.

For benchmark experiments, 235 critical configurations were selected from the ICSBEP. In the selected experiments the fissile material was MOX in 96 cases, plutonium in 55 cases and low enriched uranium for 84 cases. With only a few exceptions, the neutron spectrum was thermal. This set of configurations was investigated by TSUMAMI and TSURFER modules.
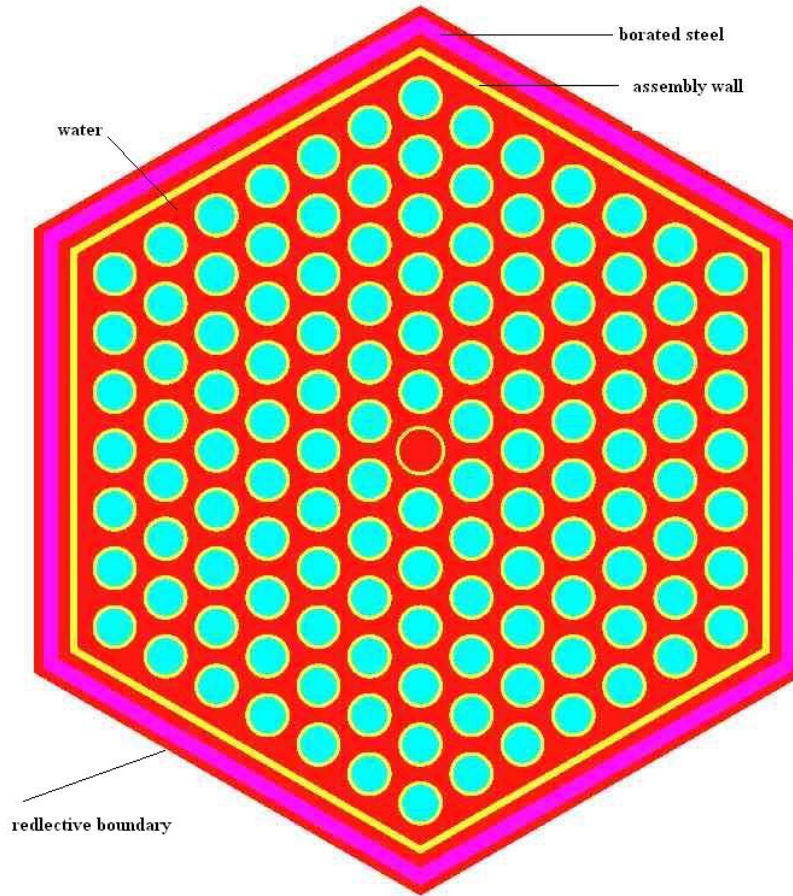
Figure 1. Horizontal cross section of the model used for the storage pool

TSUNAMI calculations

A series of criticality calculations were performed for the selected experiments by TSUMAMI-3D. It was found for all cases, that measured multiplication factor is included in the interval determined by the calculated multiplication factor ± uncertainty due to nuclear data. For storage pool with the burned fuel specified above it was found, that

$$k_{eff} = 0.88870 \quad \text{and} \quad \sigma_x = 0.6\ \%.$$

Here σ_x is standard deviation of the uncertainty due to nuclear data. The main sources of this uncertainty are the Pu-239 nubar, U-238 (n,gamma), U-235 nubar, Pu-239 fission and Pu-239 (n,gamma) cross sections. The statistical uncertainty of the Monte Carlo calculation is less by at least by one order of magnitude.

Evaluation of similarity indices between this application and the experiments by TSUNAMI-IP shows quite low degree of similarity. The c_k values range from 0.1 to the maximal value 0.82. For thermal MOX experiments this value is between 0.6 and 0.82, for the few fast MOX experiment is between 0.1 and 0.2, for thermal plutonium solution

is between 0.5 and 0.67, and for LEU experiments is between 0.3 and 0.45. It is widely considered that a number of experiments with $c_k > 0.9$ or possibly $c_k > 0.95$ is necessary for reliable determination of an upper safety limit with extrapolation to $c_k = 1.0$. It is clear that this set of experiments definitely insufficient for derivation. However, for methodological purposes a series of calculations were performed by USLSTATS, changing the minimal c_k value from 0.1 to 0.7. The results are shown on the next Table. USL-1 means the USLSTATS method 1, confidence band with administrative safety margin. The calculations were performed by the following parameters:

P = proportion of population falling above lower tolerance level, 0.999
1 - γ = confidence on fit, 0.95
α = confidence on proportion P, 0.999
Δk_m = administrative margin used to ensure subcriticality, 0.050

Minimal c_k	Number of experiments	normality	USL-1
0.1	235	Yes	0.9261
0.3	206	Yes	0.9251
0.4	168	No	0.9225
0.5	147	No	0.9092
0.6	118	Yes	0.9022
0.7	42	Yes	0.8807

Recalling that the calculated value of nuclear uncertainty is only 0.6 %, it can be seen, that application of the method would result quite restrictive safety margin.

Increasing the number of the selected experiments theoretically may increase the maximal similarity index achieved, however it is known from the literature, that c_k value higher than 0.9 can hardly be achieved [2].

Unlike the similarity index, the coverage of application by the experiments is fairly good. For most reactions of actinides, the application sensitivity is practically identical with the composite sensitivity. The completeness parameter is 0.91, requiring that for all reactions of all nuclides in all energy groups should be at least 10 experiments, which has sensitivity at least 90 % of the application sensitivity. This indicates that use of TSURFER may be useful.

TSURFER calculations

The application and experiments described above was investigated by TSURFER. The errors of measured multiplication factor were taken from the ICSBEP handbook. Unfortunately, no correlation data was available for the selected experiments, so constant correlation was assumed among measurements due to the same evaluations and zero correlation was assumed among measurements due to different evaluations. The value of this constant originally was chosen to 0.7 but it resulted a warning, that the correlation

matrix is not positive definite, so its value was changed to 0.4. Delta chi-square filtering was used with target value 1.2, which excluded 14 experiments from the analysis. Only experiments with c_k higher than 0.2 was considered, so altogether 218 experiments were analyzed. The results of the procedure are shown on the next Tables.

Initial χ2 per degrees of freedom	2.567E+00
Target χ2 per degrees of freedom	1.200E+00
Final χ2 per degrees of freedom	1.171E+00

Table 2. Results of χ2 filtering

calculated k_{eff}	prior std dev (%)	bias	adjusted k_{eff}	adjusted std dev %
0.88870	0.55207	1.140E-03	0.88756	0.17955

Table 3. Results of the adjustment procedure
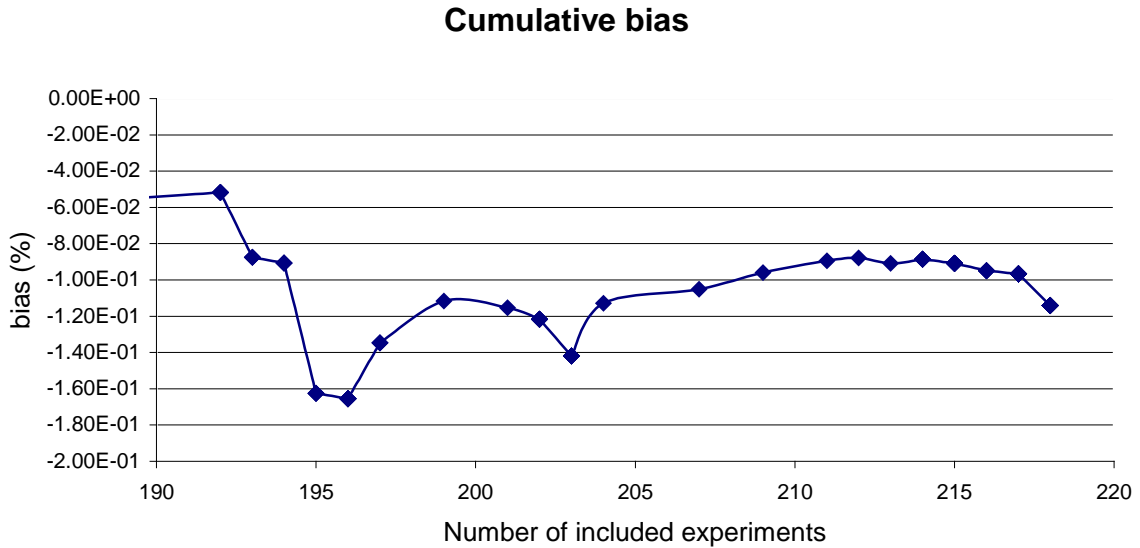
Cumulative bias

Table 4. Cumulative bias as function of included experiments

The procedure eliminated about 70 % of the uncertainties due to nuclear data. Main contributors are U-238(n,gamma), U-235 nubar, U-238(n,n'), Pu-239 fission, U-235 fission and U-235(n,gamma). The result of χ2 filtering suggests that the procedure was correct. However, the change of calculated bias with the number of included experiments shows, that the convergence was not achieved. This shortage might be eliminated by including more experiments into the analysis.

It is worthy to note, that some trial calculations show, that modifying the correlations among experiments may increase the bias from 1.14e-03 to 3.1e-03, so having correct correlation data is an important issue.

References

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[2] Evaluation of the French Haut Taux de Combustion (HTC) Critical Experiment Data, NUREG/CR-6979,ORNL/TM-2007/083, D.E. Mueller, K.R. Elam, and P.B. Fox