CRITICALITY SAFETY EVALUATIONS FOR THE CONCEPT OF SWISS PWR SPENT FUEL GEOLOGICAL REPOSITORY

A. Vasiliev¹, J. Herrero¹*, D. Rochman¹, M. Pecchia¹, H. Ferroukhi¹ and S. Caruso²

¹ Paul Scherrer Institut (PSI), Villigen PSI, Switzerland
² National Cooperative for the Disposal of Radioactive Waste (NAGRA), Wettingen, Switzerland

alexander.vasiliev@psi.ch, dimitri-alexandre.rochman@psi.ch, marco.pecchia@psi.ch, hakim.ferroukhi@psi.ch, stefano.caruso@nagra.ch

ABSTRACT

R&D works on the spent fuel criticality safety, including burnup credit, are ongoing in Switzerland in relation to the preparation of a general license application for a deep geological repository, which is led by NAGRA (Swiss National Technical Competence Centre in the field of deep geological disposal of radioactive waste) in cooperation with the Paul Scherrer Institute (PSI). The task of PSI in this joint project is deriving loading curves for a reference canister design provided by NAGRA, intended to cover, ultimately, the entire park of the fuel assemblies operated and currently stored in Switzerland as well as the component of spent fuel foreseen for the future NPP’s operation. Comparing to existing methodologies, one can characterize the approach currently chosen by PSI as a combination of the best estimate plus uncertainty (BEPU) concept with certain bounding conservative assumptions and conditions. Regarding the uncertainty assessments, the presently identified major sources of the uncertainties include the nuclear data and the spent nuclear fuel composition affected as well by the nuclear data uncertainties and also by operating conditions for every particular fuel assembly. A critical feature of the modern burnup credit methodologies is that the benchmarks available for validation of the criticality calculations were performed with fresh fuel. Therefore, it is important to consider whether the available benchmarks are representative for the final methodology application for systems with spent nuclear fuel and also accurately assess the uncertainties related to the spent fuel nuclear data. For that purpose, the benchmark-to-application system similarity assessment is under introduction into the PSI criticality safety evaluation methodology for the spent fuel geological repository, called BUCSS-R. The present paper describes the current status of the BUCSS-R methodology with the focus on its BEPU specific characteristics.

1. INTRODUCTION

From the previous scoping studies performed at NAGRA for the preliminary conceptual designs of the spent nuclear fuel (SNF) canisters for the final geological repository, it was concluded that the nuclear criticality safety cannot be guaranteed without taking credit for the SNF reactivity change with burnup, which is known in the literature as the burnup credit (BUC) approach.

* Current affiliation: ENUSA Industrias Avanzadas, Madrid, Spain
Typically the BUC applications are conditionally categorised as either only actinides credit (AC) or actinides plus fission products (AC+FP) credit. The former case basically accounts for the net reduction of the fissile material content with burnup while the later also gives credit to the accumulation of the fission products, which elevates the challenge for validation procedures. Normally, the fuel depletion calculations for BUC evaluations are done with a set of bounding parameters in terms of power density, fuel and coolant temperatures, densities, etc., so that the reactivity of the fuel at discharge for such conservative assumptions will be higher than the reactivity obtained with any possible real irradiation history. This path however was not fully adopted for the joint PSI/NAGRA BUCSS-R (BUrunp Credit System for the Swiss Reactors – Repository case) project. The approach being utilised is different because real operational data could be employed (using available CASMO/SIMULATE3 validated core follow models at PSI) for all fuel assemblies operated in Switzerland. This allows estimating the loading curves on the basis of best-estimate assessments integrated with a conservative but rational treatment of uncertainties. At present the work on two alternative ways to finalise the loading curves is ongoing at PSI: produce 95%/95% limits for the loading curves using the base methodology developed within the BUCSS-R project, or perform explicit evaluation of every operated fuel assembly based on the PSI in-house validated database of the Swiss reactors’ operation cycles, built with CASMO/SIMULATE/SNF code models.

In the present PSI BUCSS-R methodology the fuel depletion and decay simulations are performed respectively using the CASMO code and the decay module of the SERPENT code and their validation is primarily based on proprietary PIE data obtained at PSI Hot Lab. For the final step of the loading curves development, criticality calculations are performed with MCNP® (https://mcnp.lanl.gov) for models of the disposal canisters loaded with spent fuel assemblies. In order to validate the MCNP criticality calculations with a selected Nuclear Data (ND) library, a set of critical benchmark experiments from the ICSBEP Handbook [1] is in use at PSI [2].

This paper presents a representative example of the preliminary loading curves obtained for PWR fuel, which determine minimum average fuel assembly burnup required for a given original fuel enrichment of the fuel assemblies, so that the effective neutron multiplication factor \(k_{\text{eff}}\) of the canister will comply with the imposed criticality safety criterion.

One of the principle problems for routine justification of the BUC concept, especially for the AC+FP credit, is the lack of experimental data particularly appropriate for validation of the criticality calculations for spent fuel. Therefore the validation of the criticality calculations for the canister loaded with spent fuel can practically be done primary using the available criticality benchmarks with fresh UO\(_2\) and MOX fuel. At these circumstances a comprehensive uncertainty assessment, which may not be required for the conventional criticality safety evaluations (CSE) of fresh fuel, would help to justify the BUC approach application. Furthermore, in addition to the basic uncertainty quantifications, the need for assessment of a representativity of the validation benchmarks for the application case CSE becomes evident. It is also obvious that for the CSE applications the role of the nuclear data uncertainties is of paramount importance [3].

\(\dagger\) Typically, only a selected set of stable, non-volatile and strong neutron absorbers -fission products is included in AC+FP BUC evaluations. This actually leads to the situation that the considered AC+FP spent nuclear fuel compositions are most reactive (conservative) at no decay time, which obviously may not be the case for the complete FP list and also for the AC BUC option.
2. BACKGROUND ON THE BUCSS-R METHODOLOGY

2.1 Original Criticality Safety Criterion

The criticality safety criterion, applied at PSI for the preliminary evaluation of the loading curves for the disposal canisters with Swiss SNF can be presented with the following relations:

$$k_{eff|\text{Canister}}^{Bounding\ FA\ pos}(BU) + \Delta k_{eff|\text{Canister}}^{AX}(BU) + \Delta k_{eff|\text{Canister}}^{Rad}(BU) + 2\sigma_{tot}(BU) < USL = k_{eff|\text{AOA}}^{LTB} - \Delta k_{eff|\text{AOA}}^{AM} ;$$  \hspace{1cm} (1)

$$\sigma_{tot}(BU) = \sqrt{\sigma_{ND}(BU)^2 + \sigma_{BU-eff}(BU)^2 + \sigma_{OP}(BU)^2 + \sigma_{TP}^2 + \sigma_{T1/2}^2 + \sigma_{MC}^2} ;$$  \hspace{1cm} (2)

$$\sigma_{ND}(BU) = \sigma_{ND}^{CASMO}(BU) + \sigma_{ND}^{MCNP}(BU) ,$$  \hspace{1cm} (3)

where $k_{eff|\text{Canister}}^{Bounding\ FA\ pos}$ is $k_{eff}$ corresponding to the disposal canister loaded with spent fuel assemblies placed in the most penalizing positions considering the canister technological tolerances; $\Delta k_{eff|\text{Canister}}^{AX}$ and $\Delta k_{eff|\text{Canister}}^{Rad}$ are the $k_{eff}$ penalties to cover bounding axial and radial burnup profiles, respectively; USL is the Upper Subcritical Limit (see for details [4]), $\sigma_{ND}, \sigma_{BU-eff}, \sigma_{OP}, \sigma_{TP}, \sigma_{T1/2}$ and $\sigma_{MC}$ are the uncertainties at one standard deviation level, respectively for the nuclear data (ND), burnup induced changes (BU), operating conditions (OP), technological parameters (TP), decay constants (half-life) and the Monte Carlo statistical uncertainty (MC) of the criticality calculations with MCNP. The listed components of the $\sigma_{tot}(BU)$ uncertainty are assumed to be stochastic (not systematic) and uncorrelated. The resulting $\sigma_{tot}(BU)$ is further assumed to be normally distributed. Under these conditions the term $2\sigma_{tot}(BU)$ in Eq. (1) is supposed to represent 95% confidence interval for $k_{eff}$. The $\sigma_{ND}^{CASMO}$ nuclear data-related component is responsible for the $k_{eff}$ uncertainty associated with the spent fuel composition (due to the propagation of nuclear data uncertainties during depletion calculations) and the $\sigma_{ND}^{MCNP}$ component is the $k_{eff}$ uncertainty due to the nuclear data in the criticality calculations. Further details on this approximation are discussed in Section 2.3.

The $k_{eff|\text{AOA}}^{LTB}$ term stands for the Lower Tolerance Bound for $k_{eff}$ predictions for the particular Area of Applicability (AOA, here it is limited to LWR fuel) and it can be derived based on two approaches: assuming that the hypothetical population of the calculated-to-benchmark $\{k_{eff|\text{Canister}}^{Calc,b}/k_{eff|\text{Canister}}^{b}\}$ values follow the Gaussian distribution, or based on order (distribution-free) statistics. It was found in the previous studies that both approaches usually agree well [2],[4].
A drawback of the distribution-free approach is that one cannot easily apply it to arbitrary combinations of the population proportion and confidence for the LTB value. This can especially be a problem when values higher than 95%/95% are required, because such combinations would need impractically large sizes of the $[k_{\text{eff}}^{\text{catch}}/k_{\text{eff}}^b]$ samples, noting that the number of available and appropriate benchmark experiments is limited. However, the present validation database employed at PSI includes 149 benchmark cases, which is fully sufficient for the 95%/95% criterion. Details on the CSE methodology accepted at PSI, including the procedures for the LTB calculations and also ongoing studies on the methodology upgrading can be found in [5]. Finally, $\Delta k_{\text{eff}}^{AM}$ is the ‘administrative margin’, normally imposed to cover unknown uncertainties to ensure subcriticality, which is assumed here to be 0.05000 (5000pcm) in $\Delta k_{\text{eff}}$.

2.2 Calculation Models

The canister model applied in the given study describes the detailed structure of the fuel assemblies including heads, grids and rods based on the design information. The first scoping study concerned the canister loaded with the same fuel in all positions, therefore a 1/8th symmetry was selected for modelling with MCNP, as illustrated on Figure 1. Axially the fuel assembly is represented with 40 nodes with independent fuel compositions. The required SNF compositions were obtained with the dedicated ‘BOHR’ CASMO-5/SIMULATE-3 calculations [6]. The axial burnup profiles of the fuel irradiated to different average burnups were retrieved from the PSI CMSYS database which includes all burnup values per fuel assembly at every axial node of the SIMULATE3 calculations. Following standard practice [7], the approach was to choose the lowest values of all the profiles for the first and the last 9 nodes, and the highest normalized burnup values of the profiles for the remaining central nodes. The calculations were done with MCNP6 code and ENDF/B-VII.1 nuclear data library.

![Figure 1 - Radial and axial (not to scale) view of the canister model.](image)

For the radial burnup profiles within the fuel assemblies there was no operational or CMSYS data available at the time of the study (such data would be available with the upgrade of SIMULATE3 to SIMULATE5/SNF in the CMSYS models). Therefore, as an alternative solution, the publicly open information on the bounding horizontal burnup profiles reported in [8] was employed.
2.3 Calculation Uncertainties Assessments

For the sake of efficient propagation of the ND-related uncertainties in the criticality calculations with official versions of the Monte Carlo codes, like MCNP6, an in-house tool NUSS has been developed at PSI to allow stochastic sampling of the nuclear data in the ACE-formatted ND library files [9]. Results of NUSS/MCNP6 uncertainty assessments are denoted as $\sigma_{ND}^{MCNP}$. It is important to underline that the NUSS tool provides flexibility in using the ND covariances in arbitrary energy structure, can be applied to any calculation output parameter and as well allows in parallel to the UQ procedure to assess straightforward correlations between different systems/output parameters. In particular, the Pearson correlation coefficient can be computed, which is relevant for the assessment of similarities in responses of different systems to the same sort of perturbations of the nuclear data which is input for, e.g., criticality calculations. More details on the NUSS tool can be found in [10].

The nuclear data uncertainty propagation in CASMO depletion calculations, resulting in the spread of the SNF composition, was done using SHARK-X tool [9]. The obtained set of the different SNF compositions was further translated to the SERPENT decay module for the decay simulation and finally provided to the MCNP6 models of the disposal canister to compute the spread of the $k_{eff}$ values due to the spread of the SNF compositions, using the nominal ENDF/B-VII.1 ND files. That SNF-related uncertainty component of $k_{eff}$ is denoted as $\sigma_{ND}^{CASMO}$. In both cases of NUSS/MCNP6 and CASMO/SHARK-X calculations, the ENDF/B-VII.1 library covariance files in 44-groups energy structure were used [9]. Without detailed discussion on the underlying evaluations for other uncertainties, Table 1 gives a summary on the presently assessed uncertainty components listed in Section 2.1 as a function of fuel burnup and for the AC+FP case.

Table 1 - Summary on $k_{eff}^{calc}$ uncertainty components, [pcm].

<table>
<thead>
<tr>
<th>Exposure (GWD/THM)</th>
<th>$\sigma_{ND}^{CASMO}*$</th>
<th>$\sigma_{ND}^{MCNP}$*</th>
<th>$\sigma_{OP}$</th>
<th>$\sigma_{BU-eff}$</th>
<th>$\sigma_{TP}$‡</th>
<th>$\sigma_{T1/2}$</th>
<th>$\sigma_{MC}$</th>
<th>$\sigma_{tot}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>367</td>
<td>0</td>
<td>0</td>
<td>10</td>
<td>0</td>
<td>25</td>
<td>368</td>
</tr>
<tr>
<td>17.6</td>
<td>249</td>
<td>311</td>
<td>100</td>
<td>200</td>
<td>10</td>
<td>15</td>
<td>25</td>
<td>604</td>
</tr>
<tr>
<td>33.8</td>
<td>396</td>
<td>304</td>
<td>400</td>
<td>200</td>
<td>10</td>
<td>15</td>
<td>25</td>
<td>831</td>
</tr>
<tr>
<td>50.5</td>
<td>536</td>
<td>298</td>
<td>500</td>
<td>700</td>
<td>10</td>
<td>15</td>
<td>25</td>
<td>1199</td>
</tr>
<tr>
<td>61.9</td>
<td>635</td>
<td>295</td>
<td>500</td>
<td>700</td>
<td>10</td>
<td>15</td>
<td>25</td>
<td>1267</td>
</tr>
<tr>
<td>72.8</td>
<td>738</td>
<td>288</td>
<td>500</td>
<td>700</td>
<td>10</td>
<td>15</td>
<td>25</td>
<td>1339</td>
</tr>
</tbody>
</table>

It must be outlined that at present some of the provided assessments on the uncertainty components are rather preliminary and may need verifications depending on availability of required modelling information. It should be noticed that the considered uncertainty parts $\sigma_{ND}^{CASMO}$ and $\sigma_{ND}^{MCNP}$ must be correlated since the underlying nuclear data are the same for the

‡ The value was estimated in a separate study [11].
*) Values reported in [6].
independently performed estimations of the both parts. Nevertheless, by present the correlation level was not assessed. In the ideal case, all calculations should be done in a single set using the same original perturbation factors for the nuclear data in both the depletion (with SHARK-X/CASMO) and the criticality (with NUSS/MCNP) calculations. However, to simplify the simulations and data processing for the initial assessments, the ND uncertainty propagations in the depletion and criticality calculations were done independently of each other. Therefore, it has been so far conservatively assumed that both parts are fully correlated and thus the estimation of the total ND-related $\sigma_{ND}(BU)$ value was done according to Eq. (3). Also, to be on the conservative side, the total ND-related uncertainties are composed from $\sigma_{ND}^{\text{CASMO}}$ corresponding to 50,000 years of cooling and $\sigma_{ND}^{\text{MCNP}}$ corresponding to zero cooling time, since this combination gives the highest total uncertainty [6].

To illustrate the total impact of the considered burnup profile penalties and the uncertainty components, Figure 2 presents the results obtained for the case of AC+FP, for the fuel assembly with 4.9wt% enrichment.

![Figure 2 - Impact of the burnup profiles and the total uncertainty on the canister $k_{eff}$ value.](image)

2.4 Preliminary Loading Curves

The final target of the work was to address a minimal average burnup per individual fuel assembly required for full load of the disposal canister without overcoming the defined upper subcritical limit. This goal was accomplished by the development of specific loading curves for discharged spent fuel assemblies, where the initial enrichment and final burnup work as loading criteria for the disposal canister.

The development of the curve is illustrated with Figure 3 and it was done as follows: the left part of Eq. (1) is plotted as a curve depending on burnup, while the right part of Eq. (1) can be shown as a constant line corresponding to the given USL value. If the burnup dependent curve of (1), and the burnup independent USL line intersect, the burnup at the point of the intersection becomes the point on the loading curve corresponding to the given fuel enrichment. Note that due to the influence of roughly estimated dependency on burnup of the uncertainties reported in Table 1, the shapes of the curves may be difficult to approximate with simple functions like a quadratic polynomial over the whole burnup range. Figure 3 shows the results for several decay times, in the units of years [a].
If for a given enrichment the burnup dependent curve of (1) is always below the USL value, then zero burnup is shown on the loading curve.

Figure 3 - Illustration on determination of the minimum burnup required for fuel to meet USL criticality safety criterion; case AC+FP.

Finally, the preliminary loading curves defined in the above described manner are illustrated with Figure 4. From these results it becomes evident that the given canister design meets the criticality safety criterion when the credit is given to the actinides plus fission products (listed in [6]) and when the fuel assemblies are burned up to the designed burnups. The “allowed” loading region refers to the case of the canister loaded with spent fuel assemblies having the same properties. However, mixed burnup loadings can also be considered eligible for disposal if the criticality safety criterion is met (it needs verification case by case).

Figure 4 - Loading curves with all conservative effects for discharged spent fuel.
2.5 Outlook on the Obtained Results

In order to provide a more clear illustration on the obtained results and to give an idea on which additional calculation efforts could be suggested to potentially allow relaxation of the currently obtained burnup credit requirements, Figure 5 is provided below. This figure shows separately different contributions to the derived burnup requirements for the single case of 4.94wt% enrichment (the cooling times are indicated in the figure legend). Both AC (red lines) and AC+FP (blue lines) BUC options are demonstrated for three different cases:

1) “Nominal results” for the canister loaded with spent fuel with nominal BU profile, no uncertainties (σ\text{tot}(BU)) are taken into account (dashed lines),

2) The same case as #1, but the nominal burnup profiles are replaced by the bounding ones (dotted lines),

3) The same as case #2, but the uncertainties are also taken into account (continuous lines).

Figure 5 also demonstrates how the burnup credit difference between the AC+FP and only AC options is changing between the considered three cases. Note that to be on the conservative side, for the AC case the decay time corresponds to 30'000 years while for the case AC+FP the decay time is zero. It can be seen that the inclusion of the bounding burnup profiles significantly increases the difference between the cases AC and AC+FP. It also can be realised that the bounding burnup profiles bring most significant penalties (consistently with Figure 2), although the uncertainty component is also important. Thus, if one wants to refine the presently obtained loading curves, it would be recommended to start the in-depth analysis from a high-fidelity evaluation of the burnup profiles and then to focus on the most significant uncertainty components: ND combined impact (σ\text{ND}); Operation conditions (σ\text{OP}) and Burnup-induced geometry changes (σ\text{BU-eff}).

![Figure 5 - Impact of different modelling components and options on the BU limits.](image-url)
3. PROSPECTS FOR THE BUCSS-R METHODOLOGY UPGRADE

3.1 Revision of the CSE Criterion

The criticality safety criterion (1) applied within the BUCSS-R project includes the nuclear data related uncertainty component for the application system, which already makes it different from the standard PSI CSE methodology designed for fresh nuclear fuel [2],[4]. However, works on further improvement of the nuclear data uncertainties treatment are currently ongoing with the focus on the analysis of the correlations between the application system and the criticality benchmark $k_{\text{eff}}$ values [5]. To reflect the common dependence of both the application system and the benchmark systems on the same underlying nuclear data, Eq. (2) should be re-written as follows (hereafter “Bounding” is shorten to “B.”):

$$\sigma_{\text{tot}}(BU) = \sqrt{\left(\frac{k_{\text{eff}}^\text{Canister}}{k_{\text{eff}}^\text{B,F,Pos}} - k_{\text{LTB}}^\text{eff} \right)^2 (BU) + \sigma_{\text{BU-eff}}^2(BU) + \sigma_{\text{OP}}^2(BU) + \sigma_T^2 + \sigma_{T/2}^2 + \sigma_{\text{MC}}^2}, \quad (4)$$

where the term $\sigma_{\text{ND}}^2(k_{\text{eff}}^\text{Canister}) = \text{VAR}(k_{\text{eff}}^\text{Canister} - k_{\text{eff}}^\text{B,F,Pos})$ is the variance of the difference between the application case $k_{\text{eff}}^\text{Canister}$ and $k_{\text{eff}}^\text{B,F,Pos}$. This can be easily done using NUSS tool, especially in the case of the distribution-free $k_{\text{eff}}^\text{LTB}$ estimation, because then $k_{\text{eff}}^\text{LTB} = k_l$ ($l$ is the benchmark index [4]), where $k_l = \frac{k_{\text{calc},b}}{k_{\text{eff},l}}$ ($k_{\text{calc},b}$ is a calculated result and $k_{\text{eff},l}$ is the reference benchmark value), consequently $\text{VAR}(k_{\text{eff}}^\text{LTB}) = \text{VAR}(k_l)$; then, with respect to the nuclear data uncertainties,

$$\text{VAR}(k_l) = \text{VAR}(\frac{k_{\text{calc},l}}{k_{\text{eff},l}}) \approx \text{VAR}(k_{\text{calc},l}).$$

Therefore,

$$\sigma_{\text{ND}}^2(k_{\text{eff}}^\text{Canister} - k_{\text{eff}}^\text{B,F,Pos}) = \sqrt{\text{VAR}(k_{\text{eff}}^\text{Canister} - k_{\text{calc},l})} =$$

$$\sqrt{\text{VAR}\left(k_{\text{eff}}^\text{Canister} - k_{\text{eff}}^\text{B,F,Pos}\right) + \text{VAR}(k_{\text{calc},l} - 2 \cdot \text{COV}(k_{\text{eff}}^\text{Canister} - k_{\text{eff}}^\text{B,F,Pos}, k_{\text{calc},l}))} =$$

$$\sqrt{\sigma_{\text{ND}}^2(k_{\text{eff}}^\text{Canister}) + \sigma_{\text{ND}}^2(k_{\text{calc},l}) - 2r \sigma_{\text{ND}}(k_{\text{eff}}^\text{Canister}) \sigma_{\text{ND}}(k_{\text{calc},l}) \sigma_{\text{ND}}(k_{\text{eff}}^\text{B,F,Pos}) \sigma_{\text{ND}}(k_{\text{calc},l})}.$$\quad (6)

The correlation coefficient $r$

$$r = \frac{\sum_{i=1}^{N}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{N}(X_i - \bar{X})^2 \sum_{i=1}^{N}(Y_i - \bar{Y})^2}} \approx \frac{\text{COV}(X,Y)}{\sqrt{\text{VAR}(X) \cdot \text{VAR}(Y)}} = \frac{\sigma_{XY}}{\sigma_X \sigma_Y}\quad (7)$$

can be obtained based on the NUSS/MCNP calculations, when $X_i = k_{\text{eff},i}^\text{Canister}$; $Y_i = k_{\text{calc},i}^\text{Canister}$. More detailed explanations can be found in [5].

\(^\dagger\) It can be done for the Gaussian-based LTB as well, although for that case calculations of all validation benchmarks with NUSS sampled libraries are required.
### 3.2 Correlation Analysis

As an illustration, Figure 6 below shows the presently obtained values of the Pearson correlation coefficients for the $k_{eff}$ samples generated with the cross-sections perturbed with NUSS, for the canister models filled with SNF of different burnups and also for representative UO$_2$ and MOX criticality benchmarks. The applied nomenclature is following: Can-0 ÷ Can-72 – models of the canister loaded with the fuel assemblies of 4.94wt% enrichment with burnups from 0 to 72 GWd/THM; the simulated type of BUC is also indicated. The benchmark cases were taken from [1]. The cases LCT-1-1 and MCT-1-1 are given only for illustration and correspond to sequentially first benchmarks from each of UO$_2$ and MOX categories in [1]. The case LCT-51-16 corresponds to the $k^\text{LTB}|_{\text{AOA}}$ obtained with ordered statistics for 95%/98.1% combination of the population proportion and the confidence values. The bottom row in Figure 6 shows the estimated nuclear data related uncertainty values (STD) for the $k_{eff}$ results in the [pcm] units**. It is remarkable that the uncertainty of the case “Can-72/AC” is larger than the one of “Can-72/AC+FP”, despite the fact that the latter case has more ND uncertainty contributors. The reason is obviously the difference in the neutron spectrum between the SNF corresponding to the AC and AC+FP cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>Can-0</th>
<th>Can-17/AC+FP</th>
<th>Can-33/AC+FP</th>
<th>Can-50/AC+FP</th>
<th>Can-61/AC+FP</th>
<th>Can-72/AC+FP</th>
<th>Can-72/AC</th>
<th>LCT-1-1</th>
<th>MCT-1-1</th>
<th>LCT-51-16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correlation</td>
<td>1</td>
<td>0.91</td>
<td>0.83</td>
<td>0.77</td>
<td>0.74</td>
<td>0.71</td>
<td>0.73</td>
<td>0.75</td>
<td>0.38</td>
<td>0.74</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.95</td>
<td>0.92</td>
<td>0.90</td>
<td>0.87</td>
<td>0.86</td>
<td>0.69</td>
<td>0.60</td>
<td>0.66</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.97</td>
<td>0.96</td>
<td>0.94</td>
<td>0.93</td>
<td>0.63</td>
<td>0.69</td>
<td>0.57</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.97</td>
<td>0.96</td>
<td>0.94</td>
<td>0.60</td>
<td>0.73</td>
<td>0.73</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.95</td>
<td>0.95</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.95</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.57</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.62</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>1</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.48</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>0.29</td>
<td>0.60</td>
<td>0.73</td>
<td>0.75</td>
</tr>
<tr>
<td>STD, pcm</td>
<td>473</td>
<td>407</td>
<td>391</td>
<td>383</td>
<td>384</td>
<td>370</td>
<td>416</td>
<td>646</td>
<td>652</td>
<td>436</td>
</tr>
</tbody>
</table>

Figure 6 - The Pearson correlation coefficient for different systems with respect to the canister loaded with PWR fuel of 4.94wt% enrichment.

The behaviour of the correlation coefficients looks quite in line with the expectations based on the physical properties of the systems, which can be seen as an additional verification of the calculation procedures.

** These values have been updated since the publication [6], primary due to inclusion of H-1 isotope into the consideration of the ND uncertainties (previously disregarded).
3.3 Discussion on the Upgraded Methodology Implementation

By present, the test estimations of the ND-related uncertainties have only been done for the case of the PWR fuel with 4.94wt% enrichment. A comparison of the limiting burnup results as obtained with the original Eq. (2) and its updated version (4) for this case of enrichment have shown rather moderate changes in the loading curves. On average the difference between the limiting $k_{eff}$ values (left parts of Eq.(1)) is slightly less than 200pcm (based on the data from Table 1; a bit higher difference would correspond to the updated uncertainty data reported in Figure 6), the lower values correspond to the upgraded equation (4). This can be translated in up to ~1GWd/tHM gain in the limiting burnup (i.e. less burnup is required). However, the upgraded approach is obviously more accurate as compared with the original one and it has the logical feature that an increased uncertainty penalty shall be paid in the cases where no similar benchmarks are available for the methodology validation, while the penalty is reduced when benchmarks closely simulating the application case are available.

One could notice that the correlation between the systems of similar design can be very high, like it is the case for the benchmarks LCT-1-1 and LCT-51-16. If, for example, system LCT-1-1 would be an application case, while LCT-51-16 is still the benchmark corresponding to $K_{eff}^{LTB}_{AOA}$. Thus, the main uncertainty component of Eq. (4) for the fresh fuel case will be

$$\sigma_{ND}^{2} = \sigma_{MC}^{2} + \sigma_{B, FA}^{2}$$

where $\sigma_{MC}$ can be typically neglected being relatively small. In that situation

$$\sigma_{tot}^{2}(BU) \approx (646 \cdot 10^{-5})^2 + (436 \cdot 10^{-5})^2 - 2 \cdot 0.93 \cdot 646 \cdot 10^{-5} \cdot 436 \cdot 10^{-5} = 289pcm$$

which is much smaller than the individual uncertainties of both LCT-1-1 and LCT-51-16 benchmarks.

With such qualitative improvement of the calculation methodology and the criticality safety criterion, one could suppose that significant justification for potential reduction of the administrative margin can be demonstrated with the present tools and methods for CSE analysis. This goes in line with the ideas on the reduction of the administrative margin at least for the situations with very unlikely accidental conditions [12]. In relation to that, for general illustration purposes, Figure 5 also shows two horizontal USL lines corresponding to two values of the administrative margin: the conventional one of 5000pcm and, for comparison, a reduced one of 2000pcm, the latter being typically employed for accidental scenarios for LWR fuel. This illustration allows predicting the saving in the minimum burnup requirement which could be achieved provided that the administrative margin is relaxed to 2000pcm. According to Figure 5, for example for the option of AC+FP, the saving would correspond to ~12GWd/tHM (or to 13GWd/tHM, taking into account the effect of Eq. 4 discussed in the beginning of this section) which is definitely an important gain.

4. CONCLUSION

The paper summarises the current status of the criticality safety studies performed at the Paul Scherrer Institute for the spent fuel disposal canisters’ designs being elaborated at NAGRA, in the frame of the PSI/NAGRA collaboration on the concept of the final repository of the Swiss spent nuclear fuel. Potential further improvements of the BUCSS-R methodology for refinement of PWR BUC loading curves have been identified and partly discussed in the paper.
5. REFERENCES


